

1 / 46

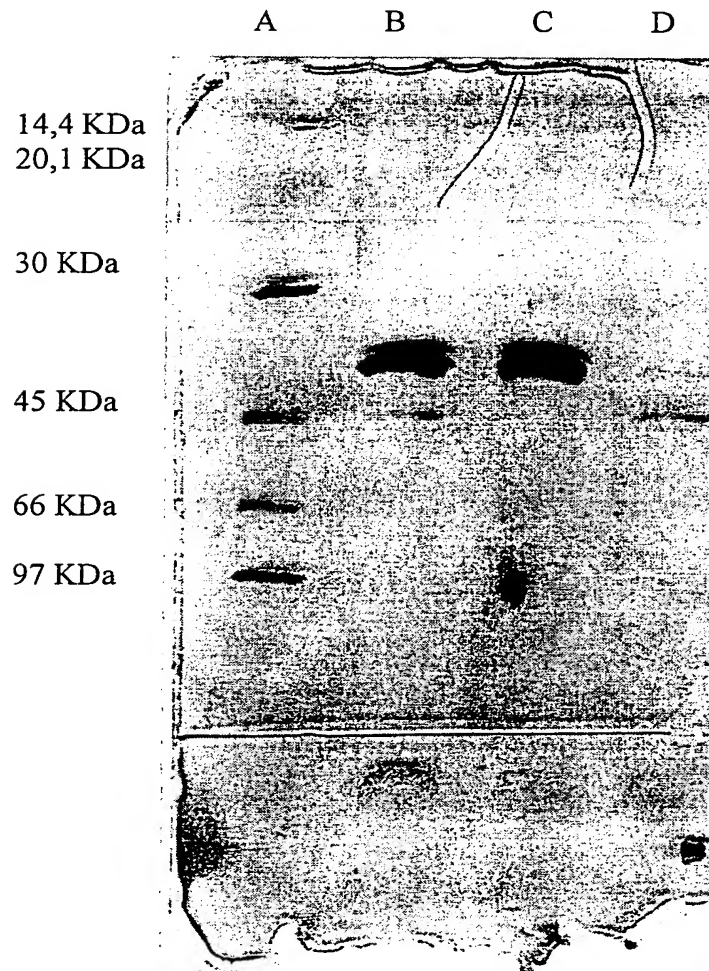


FIGURE 1

BEST AVAILABLE COPY

2 / 46

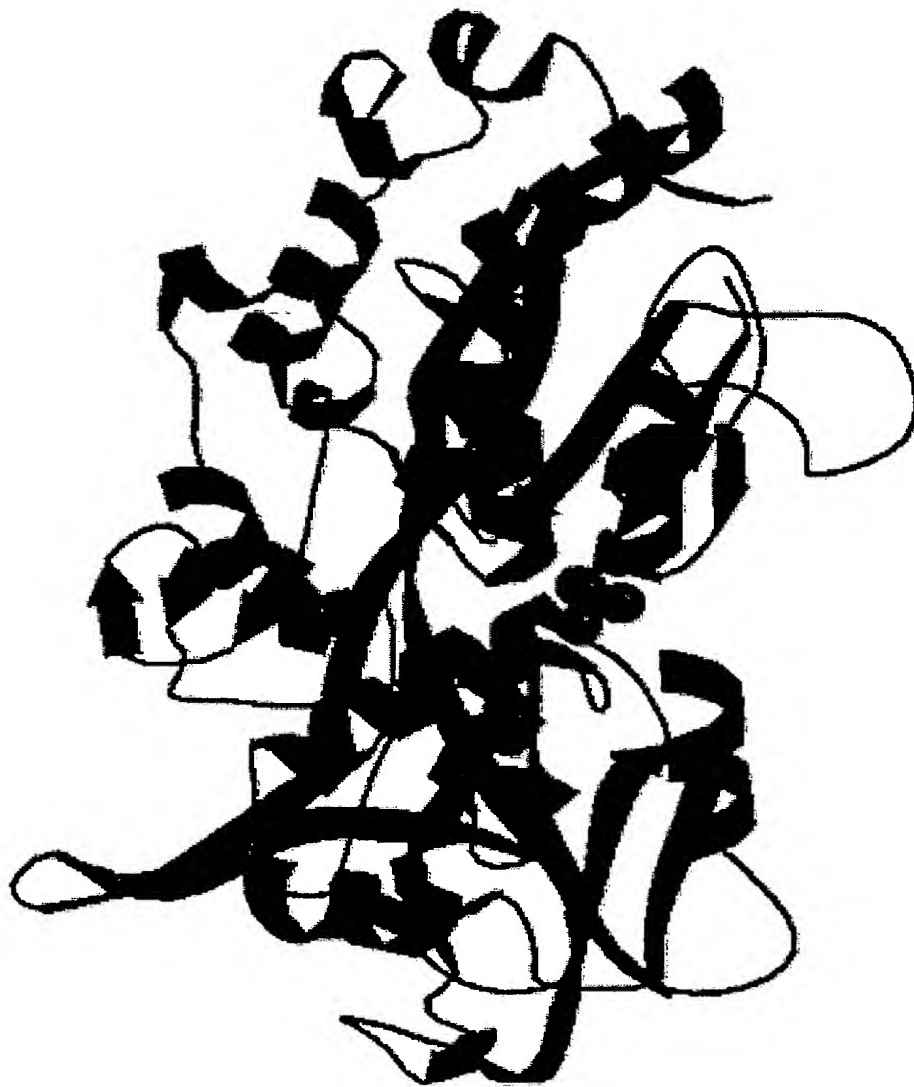


FIGURE 2

BEST AVAILABLE COPY

3 / 46

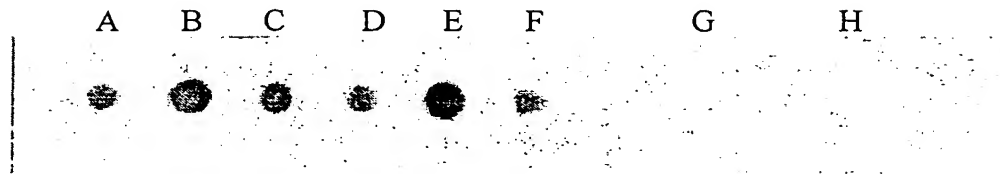


FIGURE 3

BEST AVAILABLE COPY

4 / 46

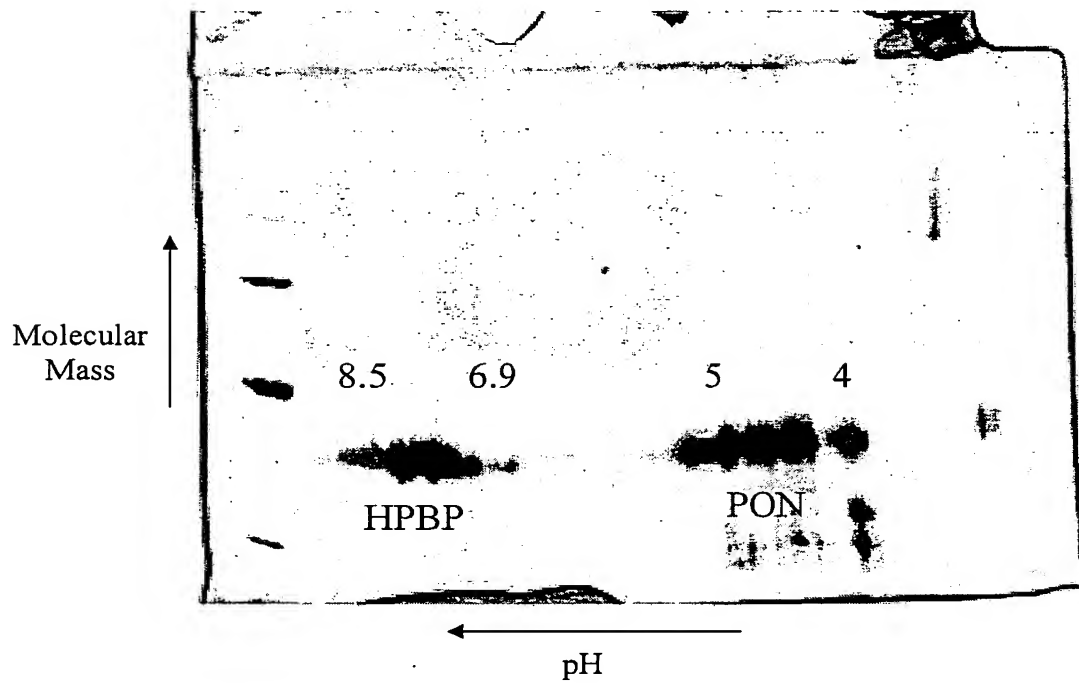


FIGURE 4

BEST AVAILABLE COPY

5 / 46

ATOM	1	CB	SER	A	1	24.666	45.653	14.370	1.00	26.15	A
ATOM	2	OG	SER	A	1	25.258	46.028	13.130	1.00	38.82	A
ATOM	3	C	SER	A	1	22.519	45.324	15.622	1.00	20.30	A
ATOM	4	O	SER	A	1	21.889	46.093	16.367	1.00	18.83	A
ATOM	5	N	SER	A	1	22.817	47.273	14.074	1.00	22.37	A
ATOM	6	CA	SER	A	1	23.146	45.831	14.317	1.00	22.87	A
ATOM	7	N	ILE	A	2	22.676	44.027	15.878	1.00	14.00	A
ATOM	8	CA	ILE	A	2	22.149	43.401	17.092	1.00	13.36	A
ATOM	9	CB	ILE	A	2	21.747	41.923	16.828	1.00	14.04	A
ATOM	10	CG2	ILE	A	2	21.536	41.191	18.155	1.00	9.05	A
ATOM	11	CG1	ILE	A	2	20.458	41.872	15.988	1.00	13.38	A
ATOM	12	CD1	ILE	A	2	20.173	40.501	15.357	1.00	14.27	A
ATOM	13	C	ILE	A	2	23.303	43.459	18.083	1.00	12.32	A
ATOM	14	O	ILE	A	2	24.376	42.890	17.847	1.00	14.26	A
ATOM	15	N	ASP	A	3	23.075	44.122	19.205	1.00	13.19	A
ATOM	16	CA	ASP	A	3	24.134	44.331	20.193	1.00	11.15	A
ATOM	17	CB	ASP	A	3	24.149	45.830	20.578	1.00	12.52	A
ATOM	18	CG	ASP	A	3	24.268	46.744	19.351	1.00	11.70	A
ATOM	19	OD1	ASP	A	3	25.289	46.618	18.642	1.00	11.97	A
ATOM	20	OD2	ASP	A	3	23.356	47.569	19.094	1.00	13.82	A
ATOM	21	C	ASP	A	3	23.981	43.508	21.456	1.00	11.88	A
ATOM	22	O	ASP	A	3	22.947	43.577	22.116	1.00	11.48	A
ATOM	23	N	GLY	A	4	25.022	42.763	21.800	1.00	9.46	A
ATOM	24	CA	GLY	A	4	24.973	41.947	23.007	1.00	10.97	A
ATOM	25	C	GLY	A	4	26.303	41.966	23.740	1.00	8.48	A
ATOM	26	O	GLY	A	4	27.314	42.413	23.200	1.00	9.87	A
ATOM	27	N	GLY	A	5	26.296	41.496	24.987	1.00	11.77	A
ATOM	28	CA	GLY	A	5	27.511	41.489	25.785	1.00	4.85	A
ATOM	29	C	GLY	A	5	27.163	41.000	27.186	1.00	8.06	A
ATOM	30	O	GLY	A	5	26.009	40.610	27.447	1.00	9.13	A
ATOM	31	N	GLY	A	6	28.144	41.021	28.089	1.00	9.80	A
ATOM	32	CA	GLY	A	6	27.898	40.589	29.458	1.00	9.86	A
ATOM	33	C	GLY	A	6	28.970	39.679	30.014	1.00	7.11	A
ATOM	34	O	GLY	A	6	30.150	40.030	30.000	1.00	8.89	A
ATOM	35	N	ALA	A	7	28.567	38.518	30.525	1.00	9.08	A
ATOM	36	CA	ALA	A	7	29.509	37.540	31.079	1.00	8.69	A
ATOM	37	CB	ALA	A	7	28.814	36.168	31.195	1.00	7.94	A
ATOM	38	C	ALA	A	7	30.811	37.363	30.277	1.00	9.69	A
ATOM	39	O	ALA	A	7	30.781	37.212	29.050	1.00	7.30	A
ATOM	40	N	THR	A	8	31.941	37.367	30.981	1.00	7.56	A
ATOM	41	CA	THR	A	8	33.236	37.135	30.338	1.00	7.21	A
ATOM	42	CB	THR	A	8	34.402	37.865	31.065	1.00	8.00	A
ATOM	43	OG1	THR	A	8	34.532	37.344	32.402	1.00	9.83	A
ATOM	44	CG2	THR	A	8	34.123	39.388	31.139	1.00	10.68	A
ATOM	45	C	THR	A	8	33.542	35.624	30.340	1.00	5.67	A
ATOM	46	O	THR	A	8	34.355	35.168	29.552	1.00	8.00	A
ATOM	47	N	LEU	A	9	32.885	34.842	31.195	1.00	6.65	A
ATOM	48	CA	LEU	A	9	33.190	33.389	31.224	1.00	9.98	A
ATOM	49	CB	LEU	A	9	32.275	32.649	32.238	1.00	10.55	A
ATOM	50	CG	LEU	A	9	32.400	31.109	32.271	1.00	11.53	A
ATOM	51	CD1	LEU	A	9	32.200	30.566	33.699	1.00	10.77	A
ATOM	52	CD2	LEU	A	9	31.356	30.503	31.300	1.00	6.94	A
ATOM	53	C	LEU	A	9	33.103	32.755	29.817	1.00	10.91	A
ATOM	54	O	LEU	A	9	33.985	31.970	29.421	1.00	9.67	A
ATOM	55	N	PRO	A	10	32.051	33.088	29.040	1.00	6.59	A
ATOM	56	CD	PRO	A	10	30.763	33.664	29.485	1.00	8.09	A
ATOM	57	CA	PRO	A	10	31.915	32.521	27.686	1.00	7.68	A
ATOM	58	CB	PRO	A	10	30.428	32.218	27.611	1.00	11.73	A
ATOM	59	CG	PRO	A	10	29.845	33.467	28.251	1.00	8.40	A
ATOM	60	C	PRO	A	10	32.317	33.504	26.579	1.00	8.72	A
ATOM	61	O	PRO	A	10	32.040	33.263	25.396	1.00	9.01	A
ATOM	62	N	GLU	A	11	33.003	34.589	26.928	1.00	5.35	A
ATOM	63	CA	GLU	A	11	33.325	35.565	25.896	1.00	8.04	A
ATOM	64	CB	GLU	A	11	33.978	36.829	26.493	1.00	12.60	A
ATOM	65	CG	GLU	A	11	35.380	36.672	27.001	1.00	21.32	A
ATOM	66	CD	GLU	A	11	35.994	38.013	27.391	1.00	26.61	A
ATOM	67	OE1	GLU	A	11	35.264	38.873	27.920	1.00	30.93	A
ATOM	68	OE2	GLU	A	11	37.203	38.202	27.176	1.00	31.32	A
ATOM	69	C	GLU	A	11	34.143	35.066	24.709	1.00	10.00	A
ATOM	70	O	GLU	A	11	33.866	35.464	23.563	1.00	8.68	A
ATOM	71	N	LYS	A	12	35.134	34.215	24.957	1.00	8.65	A
ATOM	72	CA	LYS	A	12	35.935	33.678	23.850	1.00	10.43	A
ATOM	73	CB	LYS	A	12	37.081	32.840	24.374	1.00	11.05	A
ATOM	74	CG	LYS	A	12	38.151	33.646	25.090	1.00	9.26	A
ATOM	75	CD	LYS	A	12	39.117	32.622	25.673	1.00	17.64	A

FIGURE 5

6 / 46

ATOM	76	CE	LYS	A	12	40.293	33.277	26.307	1.00	24.93	A
ATOM	77	NZ	LYS	A	12	41.298	32.237	26.600	1.00	25.96	A
ATOM	78	C	LYS	A	12	35.079	32.830	22.934	1.00	11.17	A
ATOM	79	O	LYS	A	12	35.339	32.726	21.736	1.00	8.79	A
ATOM	80	N	LEU	A	13	34.071	32.176	23.498	1.00	7.67	A
ATOM	81	CA	LEU	A	13	33.189	31.383	22.669	1.00	10.04	A
ATOM	82	CB	LEU	A	13	32.230	30.549	23.534	1.00	8.86	A
ATOM	83	CG	LEU	A	13	31.082	29.888	22.769	1.00	8.97	A
ATOM	84	CD1	LEU	A	13	31.649	28.807	21.805	1.00	12.12	A
ATOM	85	CD2	LEU	A	13	30.101	29.268	23.753	1.00	12.69	A
ATOM	86	C	LEU	A	13	32.371	32.292	21.750	1.00	9.01	A
ATOM	87	O	LEU	A	13	32.293	32.064	20.536	1.00	10.60	A
ATOM	88	N	TYR	A	14	31.761	33.329	22.305	1.00	10.47	A
ATOM	89	CA	TYR	A	14	30.920	34.195	21.482	1.00	9.03	A
ATOM	90	CB	TYR	A	14	30.029	35.087	22.352	1.00	8.38	A
ATOM	91	CG	TYR	A	14	29.091	34.293	23.253	1.00	11.48	A
ATOM	92	CD1	TYR	A	14	28.499	33.109	22.806	1.00	12.01	A
ATOM	93	CE1	TYR	A	14	27.671	32.341	23.642	1.00	10.45	A
ATOM	94	CD2	TYR	A	14	28.824	34.706	24.564	1.00	10.30	A
ATOM	95	CE2	TYR	A	14	27.998	33.948	25.403	1.00	10.35	A
ATOM	96	CZ	TYR	A	14	27.430	32.766	24.933	1.00	8.21	A
ATOM	97	OH	TYR	A	14	26.628	32.014	25.757	1.00	8.65	A
ATOM	98	C	TYR	A	14	31.715	35.036	20.489	1.00	9.67	A
ATOM	99	O	TYR	A	14	31.142	35.538	19.515	1.00	8.36	A
ATOM	100	N	LEU	A	15	33.021	35.184	20.738	1.00	8.53	A
ATOM	101	CA	LEU	A	15	33.904	35.936	19.838	1.00	9.45	A
ATOM	102	CB	LEU	A	15	35.087	36.564	20.601	1.00	8.09	A
ATOM	103	CG	LEU	A	15	34.742	37.802	21.433	1.00	14.85	A
ATOM	104	CD1	LEU	A	15	35.932	38.141	22.306	1.00	16.07	A
ATOM	105	CD2	LEU	A	15	34.364	38.990	20.510	1.00	12.61	A
ATOM	106	C	LEU	A	15	34.467	35.018	18.756	1.00	16.00	A
ATOM	107	O	LEU	A	15	35.174	35.466	17.859	1.00	16.13	A
ATOM	108	N	THR	A	16	34.178	33.729	18.848	1.00	11.70	A
ATOM	109	CA	THR	A	16	34.681	32.791	17.853	1.00	11.09	A
ATOM	110	CB	THR	A	16	34.523	31.334	18.371	1.00	11.33	A
ATOM	111	OG1	THR	A	16	35.406	31.142	19.484	1.00	13.08	A
ATOM	112	CG2	THR	A	16	34.848	30.314	17.291	1.00	11.23	A
ATOM	113	C	THR	A	16	33.906	32.997	16.549	1.00	12.10	A
ATOM	114	O	THR	A	16	32.671	32.996	16.540	1.00	12.20	A
ATOM	115	N	PRO	A	17	34.620	33.158	15.420	1.00	14.18	A
ATOM	116	CD	PRO	A	17	36.085	33.162	15.251	1.00	14.83	A
ATOM	117	CA	PRO	A	17	33.933	33.367	14.137	1.00	17.90	A
ATOM	118	CB	PRO	A	17	35.068	33.292	13.113	1.00	20.97	A
ATOM	119	CG	PRO	A	17	36.251	33.842	13.890	1.00	21.64	A
ATOM	120	C	PRO	A	17	32.830	32.341	13.854	1.00	14.42	A
ATOM	121	O	PRO	A	17	33.027	31.143	14.066	1.00	14.18	A
ATOM	122	N	ASP	A	18	31.673	32.836	13.414	1.00	15.17	A
ATOM	123	CA	ASP	A	18	30.515	32.020	13.058	1.00	19.19	A
ATOM	124	CB	ASP	A	18	30.932	30.829	12.169	1.00	23.04	A
ATOM	125	CG	ASP	A	18	31.649	31.260	10.885	1.00	30.30	A
ATOM	126	OD1	ASP	A	18	31.214	32.238	10.239	1.00	30.86	A
ATOM	127	OD2	ASP	A	18	32.645	30.599	10.511	1.00	39.65	A
ATOM	128	C	ASP	A	18	29.657	31.479	14.212	1.00	13.08	A
ATOM	129	O	ASP	A	18	28.651	30.833	13.958	1.00	13.28	A
ATOM	130	N	VAL	A	19	30.041	31.709	15.466	1.00	13.07	A
ATOM	131	CA	VAL	A	19	29.199	31.221	16.570	1.00	8.94	A
ATOM	132	CB	VAL	A	19	29.976	31.225	17.911	1.00	9.65	A
ATOM	133	CG1	VAL	A	19	29.014	31.123	19.098	1.00	11.73	A
ATOM	134	CG2	VAL	A	19	30.930	30.026	17.923	1.00	11.99	A
ATOM	135	C	VAL	A	19	27.971	32.126	16.613	1.00	11.81	A
ATOM	136	O	VAL	A	19	26.829	31.655	16.707	1.00	11.21	A
ATOM	137	N	LEU	A	20	28.198	33.434	16.567	1.00	10.93	A
ATOM	138	CA	LEU	A	20	27.077	34.363	16.486	1.00	8.58	A
ATOM	139	CB	LEU	A	20	27.439	35.730	17.084	1.00	13.44	A
ATOM	140	CG	LEU	A	20	27.677	35.767	18.601	1.00	14.24	A
ATOM	141	CD1	LEU	A	20	27.863	37.222	19.084	1.00	13.26	A
ATOM	142	CD2	LEU	A	20	26.480	35.130	19.315	1.00	11.94	A
ATOM	143	C	LEU	A	20	26.857	34.470	14.969	1.00	15.21	A
ATOM	144	O	LEU	A	20	27.836	34.550	14.196	1.00	11.72	A
ATOM	145	N	THR	A	21	25.596	34.455	14.540	1.00	14.05	A
ATOM	146	CA	THR	A	21	25.268	34.511	13.114	1.00	12.27	A
ATOM	147	CB	THR	A	21	24.006	33.653	12.865	1.00	16.46	A
ATOM	148	OG1	THR	A	21	22.966	34.044	13.774	1.00	13.53	A
ATOM	149	CG2	THR	A	21	24.326	32.173	13.121	1.00	17.80	A
ATOM	150	C	THR	A	21	25.121	35.937	12.509	1.00	14.67	A
ATOM	151	O	THR	A	21	25.452	36.928	13.148	1.00	12.04	A

FIGURE 5 (continued)

7 / 46

ATOM	152	N	ALA	A	22	24.663	36.037	11.265	1.00	12.98	A
ATOM	153	CA	ALA	A	22	24.523	37.335	10.594	1.00	12.25	A
ATOM	154	CB	ALA	A	22	23.913	37.146	9.208	1.00	15.06	A
ATOM	155	C	ALA	A	22	23.749	38.418	11.337	1.00	10.99	A
ATOM	156	O	ALA	A	22	22.688	38.174	11.916	1.00	15.12	A
ATOM	157	N	GLY	A	23	24.285	39.636	11.292	1.00	13.67	A
ATOM	158	CA	GLY	A	23	23.631	40.753	11.951	1.00	14.86	A
ATOM	159	C	GLY	A	23	24.068	41.057	13.371	1.00	14.29	A
ATOM	160	O	GLY	A	23	23.775	42.138	13.894	1.00	15.41	A
ATOM	161	N	PHE	A	24	24.760	40.116	14.001	1.00	12.44	A
ATOM	162	CA	PHE	A	24	25.238	40.283	15.363	1.00	14.48	A
ATOM	163	CB	PHE	A	24	25.424	38.899	16.020	1.00	9.89	A
ATOM	164	CG	PHE	A	24	24.156	38.276	16.527	1.00	12.35	A
ATOM	165	CD1	PHE	A	24	23.225	37.734	15.644	1.00	6.46	A
ATOM	166	CD2	PHE	A	24	23.888	38.237	17.898	1.00	12.73	A
ATOM	167	CE1	PHE	A	24	22.035	37.153	16.125	1.00	11.12	A
ATOM	168	CE2	PHE	A	24	22.695	37.662	18.397	1.00	7.42	A
ATOM	169	CZ	PHE	A	24	21.772	37.118	17.502	1.00	11.79	A
ATOM	170	C	PHE	A	24	26.584	41.030	15.444	1.00	14.36	A
ATOM	171	O	PHE	A	24	27.569	40.592	14.850	1.00	12.41	A
ATOM	172	N	ALA	A	25	26.630	42.141	16.183	1.00	14.60	A
ATOM	173	CA	ALA	A	25	27.881	42.875	16.378	1.00	13.54	A
ATOM	174	CB	ALA	A	25	27.606	44.233	17.024	1.00	15.19	A
ATOM	175	C	ALA	A	25	28.752	42.031	17.315	1.00	12.48	A
ATOM	176	O	ALA	A	25	28.240	41.155	18.023	1.00	12.61	A
ATOM	177	N	PRO	A	26	30.067	42.289	17.348	1.00	11.27	A
ATOM	178	CD	PRO	A	26	30.837	43.202	16.476	1.00	13.96	A
ATOM	179	CA	PRO	A	26	30.952	41.507	18.231	1.00	12.70	A
ATOM	180	CB	PRO	A	26	32.334	42.117	17.989	1.00	14.99	A
ATOM	181	CG	PRO	A	26	32.241	42.582	16.519	1.00	19.22	A
ATOM	182	C	PRO	A	26	30.536	41.602	19.699	1.00	10.57	A
ATOM	183	O	PRO	A	26	30.222	42.681	20.192	1.00	10.54	A
ATOM	184	N	TYR	A	27	30.529	40.456	20.367	1.00	8.04	A
ATOM	185	CA	TYR	A	27	30.161	40.345	21.793	1.00	9.13	A
ATOM	186	CB	TYR	A	27	30.294	38.886	22.231	1.00	8.74	A
ATOM	187	CG	TYR	A	27	29.824	38.612	23.648	1.00	5.12	A
ATOM	188	CD1	TYR	A	27	28.469	38.512	23.938	1.00	6.81	A
ATOM	189	CE1	TYR	A	27	28.024	38.224	25.247	1.00	9.00	A
ATOM	190	CD2	TYR	A	27	30.741	38.423	24.682	1.00	5.70	A
ATOM	191	CE2	TYR	A	27	30.310	38.131	25.992	1.00	7.78	A
ATOM	192	CZ	TYR	A	27	28.948	38.032	26.259	1.00	9.36	A
ATOM	193	OH	TYR	A	27	28.502	37.709	27.532	1.00	8.37	A
ATOM	194	C	TYR	A	27	31.081	41.207	22.675	1.00	10.49	A
ATOM	195	O	TYR	A	27	32.297	41.207	22.494	1.00	9.91	A
ATOM	196	N	ILE	A	28	30.510	41.931	23.635	1.00	8.97	A
ATOM	197	CA	ILE	A	28	31.324	42.765	24.517	1.00	12.31	A
ATOM	198	CB	ILE	A	28	30.801	44.225	24.521	1.00	13.61	A
ATOM	199	CG2	ILE	A	28	31.657	45.098	25.459	1.00	13.95	A
ATOM	200	CG1	ILE	A	28	30.871	44.793	23.095	1.00	11.91	A
ATOM	201	CD1	ILE	A	28	30.192	46.146	22.915	1.00	12.92	A
ATOM	202	C	ILE	A	28	31.333	42.191	25.942	1.00	13.14	A
ATOM	203	O	ILE	A	28	30.315	42.189	26.622	1.00	8.79	A
ATOM	204	N	GLY	A	29	32.499	41.706	26.373	1.00	13.23	A
ATOM	205	CA	GLY	A	29	32.630	41.105	27.695	1.00	15.83	A
ATOM	206	C	GLY	A	29	32.868	42.127	28.791	1.00	16.10	A
ATOM	207	O	GLY	A	29	33.915	42.794	28.826	1.00	12.27	A
ATOM	208	N	THR	A	30	31.900	42.234	29.697	1.00	8.70	A
ATOM	209	CA	THR	A	30	31.966	43.200	30.783	1.00	10.71	A
ATOM	210	CB	THR	A	30	31.061	44.442	30.473	1.00	11.83	A
ATOM	211	OG1	THR	A	30	29.703	44.014	30.222	1.00	16.91	A
ATOM	212	CG2	THR	A	30	31.607	45.235	29.249	1.00	8.83	A
ATOM	213	C	THR	A	30	31.538	42.640	32.147	1.00	11.78	A
ATOM	214	O	THR	A	30	31.532	43.378	33.135	1.00	11.34	A
ATOM	215	N	GLY	A	31	31.187	41.352	32.210	1.00	10.41	A
ATOM	216	CA	GLY	A	31	30.729	40.789	33.473	1.00	8.40	A
ATOM	217	C	GLY	A	31	29.208	40.604	33.467	1.00	9.64	A
ATOM	218	O	GLY	A	31	28.478	41.396	32.862	1.00	8.01	A
ATOM	219	N	SER	A	32	28.718	39.566	34.138	1.00	7.93	A
ATOM	220	CA	SER	A	32	27.274	39.297	34.143	1.00	4.39	A
ATOM	221	CB	SER	A	32	26.961	37.954	34.832	1.00	2.86	A
ATOM	222	OG	SER	A	32	27.538	36.876	34.125	1.00	6.73	A
ATOM	223	C	SER	A	32	26.440	40.386	34.793	1.00	7.61	A
ATOM	224	O	SER	A	32	25.321	40.626	34.354	1.00	9.70	A
ATOM	225	N	GLY	A	33	26.984	41.052	35.811	1.00	8.20	A
ATOM	226	CA	GLY	A	33	26.256	42.121	36.506	1.00	6.91	A

FIGURE 5 (continued)

8 / 46

ATOM	227	C	GLY	A	33	25.942	43.235	35.524	1.00	9.16	A
ATOM	228	O	GLY	A	33	24.799	43.708	35.429	1.00	9.95	A
ATOM	229	N	LYS	A	34	26.943	43.633	34.749	1.00	10.60	A
ATOM	230	CA	LYS	A	34	26.710	44.681	33.758	1.00	8.52	A
ATOM	231	CB	LYS	A	34	28.040	45.240	33.250	1.00	7.07	A
ATOM	232	CG	LYS	A	34	28.667	46.220	34.250	1.00	12.80	A
ATOM	233	CD	LYS	A	34	29.957	46.854	33.703	1.00	10.66	A
ATOM	234	CE	LYS	A	34	30.597	47.768	34.748	1.00	10.90	A
ATOM	235	NZ	LYS	A	34	29.700	48.890	35.066	1.00	23.47	A
ATOM	236	C	LYS	A	34	25.848	44.201	32.601	1.00	12.94	A
ATOM	237	O	LYS	A	34	25.070	44.977	32.043	1.00	9.59	A
ATOM	238	N	GLY	A	35	25.983	42.928	32.236	1.00	9.69	A
ATOM	239	CA	GLY	A	35	25.158	42.386	31.162	1.00	7.50	A
ATOM	240	C	GLY	A	35	23.677	42.414	31.542	1.00	9.68	A
ATOM	241	O	GLY	A	35	22.831	42.767	30.717	1.00	9.00	A
ATOM	242	N	LYS	A	36	23.340	42.077	32.787	1.00	8.56	A
ATOM	243	CA	LYS	A	36	21.929	42.089	33.173	1.00	7.26	A
ATOM	244	CB	LYS	A	36	21.709	41.393	34.533	1.00	9.15	A
ATOM	245	CG	LYS	A	36	21.954	39.861	34.445	1.00	5.28	A
ATOM	246	CD	LYS	A	36	21.394	39.069	35.662	1.00	6.85	A
ATOM	247	CE	LYS	A	36	21.990	39.576	36.986	1.00	11.53	A
ATOM	248	NZ	LYS	A	36	21.397	38.945	38.221	1.00	11.99	A
ATOM	249	C	LYS	A	36	21.409	43.527	33.204	1.00	11.18	A
ATOM	250	O	LYS	A	36	20.311	43.787	32.724	1.00	14.03	A
ATOM	251	N	ILE	A	37	22.190	44.459	33.749	1.00	9.12	A
ATOM	252	CA	ILE	A	37	21.752	45.854	33.766	1.00	11.15	A
ATOM	253	CB	ILE	A	37	22.778	46.779	34.462	1.00	10.46	A
ATOM	254	CG2	ILE	A	37	22.424	48.252	34.197	1.00	11.32	A
ATOM	255	CG1	ILE	A	37	22.774	46.522	35.972	1.00	9.50	A
ATOM	256	CD1	ILE	A	37	24.024	47.029	36.669	1.00	15.62	A
ATOM	257	C	ILE	A	37	21.563	46.368	32.325	1.00	11.78	A
ATOM	258	O	ILE	A	37	20.570	47.017	32.018	1.00	11.36	A
ATOM	259	N	ALA	A	38	22.518	46.071	31.452	1.00	9.31	A
ATOM	260	CA	ALA	A	38	22.438	46.539	30.063	1.00	10.19	A
ATOM	261	CB	ALA	A	38	23.650	46.016	29.269	1.00	10.93	A
ATOM	262	C	ALA	A	38	21.129	46.102	29.375	1.00	9.69	A
ATOM	263	O	ALA	A	38	20.447	46.899	28.712	1.00	8.41	A
ATOM	264	N	PHE	A	39	20.771	44.831	29.541	1.00	8.70	A
ATOM	265	CA	PHE	A	39	19.566	44.327	28.914	1.00	9.40	A
ATOM	266	CB	PHE	A	39	19.549	42.787	28.888	1.00	9.06	A
ATOM	267	CG	PHE	A	39	18.287	42.214	28.270	1.00	7.16	A
ATOM	268	CD1	PHE	A	39	18.223	41.953	26.896	1.00	8.56	A
ATOM	269	CD2	PHE	A	39	17.146	42.000	29.051	1.00	8.19	A
ATOM	270	CE1	PHE	A	39	17.035	41.481	26.306	1.00	9.12	A
ATOM	271	CE2	PHE	A	39	15.947	41.530	28.479	1.00	9.01	A
ATOM	272	CZ	PHE	A	39	15.888	41.269	27.101	1.00	8.28	A
ATOM	273	C	PHE	A	39	18.304	44.790	29.608	1.00	12.15	A
ATOM	274	O	PHE	A	39	17.398	45.313	28.972	1.00	10.76	A
ATOM	275	N	LEU	A	40	18.246	44.602	30.920	1.00	8.71	A
ATOM	276	CA	LEU	A	40	17.034	44.938	31.678	1.00	8.94	A
ATOM	277	CB	LEU	A	40	17.204	44.513	33.144	1.00	7.80	A
ATOM	278	CG	LEU	A	40	17.342	43.005	33.400	1.00	10.06	A
ATOM	279	CD1	LEU	A	40	17.809	42.781	34.887	1.00	6.45	A
ATOM	280	CD2	LEU	A	40	16.006	42.296	33.132	1.00	12.55	A
ATOM	281	C	LEU	A	40	16.626	46.403	31.632	1.00	10.63	A
ATOM	282	O	LEU	A	40	15.430	46.730	31.629	1.00	11.89	A
ATOM	283	N	GLU	A	41	17.604	47.291	31.586	1.00	10.88	A
ATOM	284	CA	GLU	A	41	17.294	48.717	31.551	1.00	9.10	A
ATOM	285	CB	GLU	A	41	18.053	49.436	32.669	1.00	13.20	A
ATOM	286	CG	GLU	A	41	17.802	48.829	34.036	1.00	11.00	A
ATOM	287	CD	GLU	A	41	18.671	49.429	35.131	1.00	22.54	A
ATOM	288	OE1	GLU	A	41	18.975	48.713	36.103	1.00	27.36	A
ATOM	289	OE2	GLU	A	41	19.037	50.616	35.043	1.00	22.49	A
ATOM	290	C	GLU	A	41	17.633	49.361	30.218	1.00	12.72	A
ATOM	291	O	GLU	A	41	17.505	50.576	30.066	1.00	13.60	A
ATOM	292	N	ASN	A	42	18.010	48.537	29.238	1.00	11.74	A
ATOM	293	CA	ASN	A	42	18.463	49.008	27.923	1.00	11.79	A
ATOM	294	CB	ASN	A	42	17.322	49.494	27.022	1.00	14.08	A
ATOM	295	CG	ASN	A	42	17.824	49.897	25.642	1.00	16.54	A
ATOM	296	OD1	ASN	A	42	18.885	49.428	25.189	1.00	15.67	A
ATOM	297	ND2	ASN	A	42	17.076	50.763	24.960	1.00	14.22	A
ATOM	298	C	ASN	A	42	19.486	50.126	28.091	1.00	16.68	A
ATOM	299	O	ASN	A	42	19.300	51.260	27.631	1.00	14.27	A
ATOM	300	N	SER	A	43	20.578	49.789	28.767	1.00	14.51	A

FIGURE 5 (continued)

9 / 46

ATOM	301	CA	SER	A	43	21.665	50.740	29.001	1.00	14.54	A
ATOM	302	CB	SER	A	43	21.920	50.874	30.520	1.00	19.90	A
ATOM	303	OG	SER	A	43	20.922	51.662	31.162	1.00	26.22	A
ATOM	304	C	SER	A	43	22.965	50.327	28.302	1.00	13.78	A
ATOM	305	O	SER	A	43	23.790	49.633	28.891	1.00	10.60	A
ATOM	306	N	TYR	A	44	23.168	50.755	27.056	1.00	9.73	A
ATOM	307	CA	TYR	A	44	24.396	50.401	26.361	1.00	10.86	A
ATOM	308	CB	TYR	A	44	24.330	50.880	24.904	1.00	10.54	A
ATOM	309	CG	TYR	A	44	25.414	50.311	24.034	1.00	12.22	A
ATOM	310	CD1	TYR	A	44	26.631	50.983	23.857	1.00	12.57	A
ATOM	311	CE1	TYR	A	44	27.625	50.469	23.011	1.00	10.91	A
ATOM	312	CD2	TYR	A	44	25.217	49.106	23.357	1.00	10.34	A
ATOM	313	CE2	TYR	A	44	26.201	48.587	22.517	1.00	11.21	A
ATOM	314	CZ	TYR	A	44	27.394	49.267	22.347	1.00	14.12	A
ATOM	315	OH	TYR	A	44	28.357	48.725	21.524	1.00	11.54	A
ATOM	316	C	TYR	A	44	25.650	50.971	27.026	1.00	8.02	A
ATOM	317	O	TYR	A	44	26.775	50.515	26.756	1.00	10.36	A
ATOM	318	N	ASN	A	45	25.484	51.941	27.917	1.00	8.55	A
ATOM	319	CA	ASN	A	45	26.657	52.547	28.535	1.00	14.36	A
ATOM	320	CB	ASN	A	45	26.271	53.811	29.337	1.00	8.69	A
ATOM	321	CG	ASN	A	45	25.707	53.503	30.708	1.00	11.69	A
ATOM	322	OD1	ASN	A	45	25.048	52.488	30.910	1.00	13.56	A
ATOM	323	ND2	ASN	A	45	25.934	54.411	31.655	1.00	14.48	A
ATOM	324	C	ASN	A	45	27.423	51.535	29.388	1.00	13.91	A
ATOM	325	O	ASN	A	45	28.573	51.781	29.755	1.00	11.13	A
ATOM	326	N	GLN	A	46	26.788	50.393	29.681	1.00	8.83	A
ATOM	327	CA	GLN	A	46	27.462	49.337	30.435	1.00	11.62	A
ATOM	328	CB	GLN	A	46	26.421	48.390	31.080	1.00	10.13	A
ATOM	329	CG	GLN	A	46	25.487	49.076	32.083	1.00	14.66	A
ATOM	330	CD	GLN	A	46	26.259	49.792	33.170	1.00	18.72	A
ATOM	331	OE1	GLN	A	46	26.983	49.165	33.937	1.00	18.65	A
ATOM	332	NE2	GLN	A	46	26.133	51.116	33.228	1.00	16.99	A
ATOM	333	C	GLN	A	46	28.408	48.543	29.491	1.00	10.06	A
ATOM	334	O	GLN	A	46	29.275	47.818	29.956	1.00	10.43	A
ATOM	335	N	PHE	A	47	28.232	48.691	28.174	1.00	8.72	A
ATOM	336	CA	PHE	A	47	29.055	48.025	27.148	1.00	7.46	A
ATOM	337	CB	PHE	A	47	28.191	47.487	25.992	1.00	7.56	A
ATOM	338	CG	PHE	A	47	27.271	46.349	26.366	1.00	12.11	A
ATOM	339	CD1	PHE	A	47	27.433	45.651	27.559	1.00	11.35	A
ATOM	340	CD2	PHE	A	47	26.268	45.945	25.474	1.00	14.21	A
ATOM	341	CE1	PHE	A	47	26.616	44.567	27.861	1.00	9.31	A
ATOM	342	CE2	PHE	A	47	25.442	44.859	25.761	1.00	9.84	A
ATOM	343	CZ	PHE	A	47	25.617	44.167	26.959	1.00	10.19	A
ATOM	344	C	PHE	A	47	30.053	48.988	26.484	1.00	12.94	A
ATOM	345	O	PHE	A	47	31.109	48.580	26.022	1.00	14.11	A
ATOM	346	N	GLY	A	48	29.677	50.257	26.378	1.00	11.49	A
ATOM	347	CA	GLY	A	48	30.551	51.222	25.731	1.00	13.51	A
ATOM	348	C	GLY	A	48	30.027	52.642	25.833	1.00	15.44	A
ATOM	349	O	GLY	A	48	28.999	52.908	26.459	1.00	16.60	A
ATOM	350	N	THR	A	49	30.722	53.566	25.187	1.00	14.37	A
ATOM	351	CA	THR	A	49	30.333	54.967	25.256	1.00	13.58	A
ATOM	352	CB	THR	A	49	31.576	55.843	25.161	1.00	14.46	A
ATOM	353	OG1	THR	A	49	32.234	55.567	23.924	1.00	15.00	A
ATOM	354	CG2	THR	A	49	32.558	55.524	26.322	1.00	13.17	A
ATOM	355	C	THR	A	49	29.301	55.436	24.216	1.00	14.30	A
ATOM	356	O	THR	A	49	28.716	56.511	24.370	1.00	12.47	A
ATOM	357	N	ASN	A	50	29.062	54.659	23.162	1.00	13.09	A
ATOM	358	CA	ASN	A	50	28.076	55.116	22.173	1.00	14.85	A
ATOM	359	CB	ASN	A	50	28.324	54.519	20.785	1.00	15.63	A
ATOM	360	CG	ASN	A	50	27.379	55.096	19.739	1.00	18.88	A
ATOM	361	OD1	ASN	A	50	26.472	55.883	20.059	1.00	19.28	A
ATOM	362	ND2	ASN	A	50	27.574	54.707	18.489	1.00	19.28	A
ATOM	363	C	ASN	A	50	26.669	54.751	22.615	1.00	14.82	A
ATOM	364	O	ASN	A	50	26.099	53.739	22.187	1.00	14.58	A
ATOM	365	N	THR	A	51	26.097	55.608	23.443	1.00	13.25	A
ATOM	366	CA	THR	A	51	24.782	55.377	23.988	1.00	15.77	A
ATOM	367	CB	THR	A	51	24.595	56.210	25.242	1.00	17.96	A
ATOM	368	OG1	THR	A	51	24.937	57.574	24.973	1.00	16.18	A
ATOM	369	CG2	THR	A	51	25.506	55.684	26.332	1.00	18.64	A
ATOM	370	C	THR	A	51	23.581	55.539	23.053	1.00	18.71	A
ATOM	371	O	THR	A	51	22.440	55.436	23.512	1.00	19.68	A
ATOM	372	N	THR	A	52	23.820	55.795	21.761	1.00	16.82	A
ATOM	373	CA	THR	A	52	22.702	55.865	20.827	1.00	19.67	A
ATOM	374	CB	THR	A	52	23.017	56.666	19.524	1.00	22.55	A
ATOM	375	OG1	THR	A	52	24.028	56.006	18.744	1.00	22.57	A

FIGURE 5 (continued)

10 / 46

ATOM	376	CG2	THR	A	52	23.460	58.081	19.875	1.00	21.07	A
ATOM	377	C	THR	A	52	22.342	54.428	20.446	1.00	17.92	A
ATOM	378	O	THR	A	52	21.270	54.175	19.905	1.00	17.96	A
ATOM	379	N	LYS	A	53	23.238	53.488	20.740	1.00	14.41	A
ATOM	380	CA	LYS	A	53	22.978	52.080	20.427	1.00	12.53	A
ATOM	381	CB	LYS	A	53	24.292	51.292	20.406	1.00	14.33	A
ATOM	382	CG	LYS	A	53	25.207	51.573	19.213	1.00	17.93	A
ATOM	383	CD	LYS	A	53	26.478	50.731	19.324	1.00	18.20	A
ATOM	384	CE	LYS	A	53	27.477	51.052	18.214	1.00	21.01	A
ATOM	385	NZ	LYS	A	53	26.908	50.784	16.865	1.00	22.67	A
ATOM	386	C	LYS	A	53	22.045	51.470	21.474	1.00	12.72	A
ATOM	387	O	LYS	A	53	22.075	51.869	22.635	1.00	11.93	A
ATOM	388	N	ASP	A	54	21.223	50.499	21.064	1.00	13.58	A
ATOM	389	CA	ASP	A	54	20.298	49.826	21.982	1.00	10.96	A
ATOM	390	CB	ASP	A	54	18.887	49.745	21.380	1.00	12.81	A
ATOM	391	CG	ASP	A	54	18.249	51.107	21.218	1.00	19.07	A
ATOM	392	OD1	ASP	A	54	18.010	51.529	20.059	1.00	17.31	A
ATOM	393	OD2	ASP	A	54	17.997	51.759	22.260	1.00	15.46	A
ATOM	394	C	ASP	A	54	20.819	48.416	22.246	1.00	8.44	A
ATOM	395	O	ASP	A	54	21.505	47.837	21.407	1.00	14.56	A
ATOM	396	N	VAL	A	55	20.485	47.875	23.411	1.00	12.75	A
ATOM	397	CA	VAL	A	55	20.919	46.541	23.799	1.00	12.22	A
ATOM	398	CB	VAL	A	55	21.150	46.486	25.328	1.00	7.89	A
ATOM	399	CG1	VAL	A	55	21.596	45.057	25.775	1.00	7.35	A
ATOM	400	CG2	VAL	A	55	22.229	47.518	25.707	1.00	6.23	A
ATOM	401	C	VAL	A	55	19.840	45.540	23.386	1.00	9.36	A
ATOM	402	O	VAL	A	55	18.659	45.768	23.630	1.00	11.95	A
ATOM	403	N	HIS	A	56	20.258	44.441	22.755	1.00	9.82	A
ATOM	404	CA	HIS	A	56	19.323	43.432	22.285	1.00	8.89	A
ATOM	405	CB	HIS	A	56	19.552	43.218	20.782	1.00	8.33	A
ATOM	406	CG	HIS	A	56	19.455	44.485	19.985	1.00	9.48	A
ATOM	407	CD2	HIS	A	56	20.414	45.264	19.430	1.00	11.14	A
ATOM	408	ND1	HIS	A	56	18.255	45.121	19.738	1.00	13.82	A
ATOM	409	CE1	HIS	A	56	18.483	46.236	19.064	1.00	12.14	A
ATOM	410	NE2	HIS	A	56	19.783	46.345	18.866	1.00	12.83	A
ATOM	411	C	HIS	A	56	19.389	42.097	23.033	1.00	9.87	A
ATOM	412	O	HIS	A	56	18.419	41.331	23.039	1.00	8.84	A
ATOM	413	N	TRP	A	57	20.531	41.797	23.649	1.00	10.03	A
ATOM	414	CA	TRP	A	57	20.618	40.535	24.385	1.00	12.07	A
ATOM	415	CB	TRP	A	57	20.753	39.340	23.430	1.00	7.72	A
ATOM	416	CG	TRP	A	57	22.078	39.288	22.673	1.00	9.96	A
ATOM	417	CD2	TRP	A	57	23.188	38.398	22.935	1.00	8.55	A
ATOM	418	CE2	TRP	A	57	24.161	38.642	21.945	1.00	7.37	A
ATOM	419	CE3	TRP	A	57	23.442	37.413	23.914	1.00	9.79	A
ATOM	420	CD1	TRP	A	57	22.430	40.021	21.570	1.00	9.43	A
ATOM	421	NE1	TRP	A	57	23.685	39.637	21.124	1.00	7.89	A
ATOM	422	CZ2	TRP	A	57	25.381	37.936	21.895	1.00	8.66	A
ATOM	423	CZ3	TRP	A	57	24.647	36.713	23.862	1.00	7.59	A
ATOM	424	CH2	TRP	A	57	25.605	36.982	22.852	1.00	13.66	A
ATOM	425	C	TRP	A	57	21.830	40.575	25.286	1.00	9.35	A
ATOM	426	O	TRP	A	57	22.648	41.481	25.179	1.00	9.06	A
ATOM	427	N	ALA	A	58	21.945	39.579	26.159	1.00	6.35	A
ATOM	428	CA	ALA	A	58	23.081	39.523	27.061	1.00	8.26	A
ATOM	429	CB	ALA	A	58	22.755	40.280	28.362	1.00	10.03	A
ATOM	430	C	ALA	A	58	23.471	38.101	27.407	1.00	7.97	A
ATOM	431	O	ALA	A	58	22.638	37.207	27.401	1.00	9.27	A
ATOM	432	N	GLY	A	59	24.749	37.908	27.702	1.00	9.58	A
ATOM	433	CA	GLY	A	59	25.213	36.608	28.184	1.00	7.09	A
ATOM	434	C	GLY	A	59	25.342	36.791	29.695	1.00	9.23	A
ATOM	435	O	GLY	A	59	25.779	37.846	30.159	1.00	10.14	A
ATOM	436	N	SER	A	60	24.938	35.801	30.484	1.00	5.73	A
ATOM	437	CA	SER	A	60	25.058	35.917	31.938	1.00	5.95	A
ATOM	438	CB	SER	A	60	23.815	36.613	32.535	1.00	10.17	A
ATOM	439	OG	SER	A	60	23.896	36.707	33.966	1.00	9.12	A
ATOM	440	C	SER	A	60	25.161	34.540	32.566	1.00	8.54	A
ATOM	441	O	SER	A	60	24.437	33.632	32.146	1.00	9.12	A
ATOM	442	N	ASP	A	61	26.067	34.376	33.536	1.00	9.30	A
ATOM	443	CA	ASP	A	61	26.132	33.124	34.292	1.00	8.23	A
ATOM	444	CB	ASP	A	61	27.543	32.485	34.381	1.00	6.13	A
ATOM	445	CG	ASP	A	61	28.600	33.266	33.649	1.00	13.41	A
ATOM	446	OD1	ASP	A	61	28.869	32.961	32.449	1.00	10.15	A
ATOM	447	OD2	ASP	A	61	29.150	34.191	34.281	1.00	13.11	A
ATOM	448	C	ASP	A	61	25.597	33.456	35.710	1.00	10.77	A
ATOM	449	O	ASP	A	61	25.818	32.716	36.658	1.00	11.14	A
ATOM	450	N	SER	A	62	24.914	34.595	35.833	1.00	7.59	A
ATOM	451	CA	SER	A	62	24.213	34.995	37.067	1.00	10.29	A

FIGURE 5 (continued)

11 / 46

ATOM	452	CB	SER	A	62	24.522	36.437	37.497	1.00	11.42	A
ATOM	453	OG	SER	A	62	23.631	36.832	38.549	1.00	11.94	A
ATOM	454	C	SER	A	62	22.721	34.944	36.706	1.00	10.70	A
ATOM	455	O	SER	A	62	22.274	35.605	35.745	1.00	9.88	A
ATOM	456	N	LYS	A	63	21.944	34.168	37.449	1.00	8.95	A
ATOM	457	CA	LYS	A	63	20.519	34.089	37.137	1.00	10.67	A
ATOM	458	CB	LYS	A	63	19.834	32.996	37.959	1.00	16.43	A
ATOM	459	CG	LYS	A	63	20.046	31.605	37.461	1.00	15.34	A
ATOM	460	CD	LYS	A	63	19.148	30.619	38.201	1.00	19.94	A
ATOM	461	CE	LYS	A	63	17.702	30.671	37.728	1.00	16.96	A
ATOM	462	NZ	LYS	A	63	16.903	29.498	38.239	1.00	14.00	A
ATOM	463	C	LYS	A	63	19.786	35.392	37.399	1.00	12.40	A
ATOM	464	O	LYS	A	63	20.192	36.183	38.257	1.00	10.37	A
ATOM	465	N	LEU	A	64	18.699	35.604	36.659	1.00	7.10	A
ATOM	466	CA	LEU	A	64	17.863	36.778	36.842	1.00	9.01	A
ATOM	467	CB	LEU	A	64	16.824	36.871	35.716	1.00	6.27	A
ATOM	468	CG	LEU	A	64	17.447	37.378	34.405	1.00	7.74	A
ATOM	469	CD1	LEU	A	64	16.586	37.016	33.190	1.00	8.96	A
ATOM	470	CD2	LEU	A	64	17.619	38.883	34.510	1.00	9.78	A
ATOM	471	C	LEU	A	64	17.168	36.569	38.197	1.00	10.06	A
ATOM	472	O	LEU	A	64	16.712	35.465	38.508	1.00	11.86	A
ATOM	473	N	THR	A	65	17.120	37.614	39.012	1.00	6.99	A
ATOM	474	CA	THR	A	65	16.503	37.481	40.334	1.00	11.54	A
ATOM	475	CB	THR	A	65	17.097	38.472	41.341	1.00	13.33	A
ATOM	476	OG1	THR	A	65	16.736	39.811	40.952	1.00	13.29	A
ATOM	477	CG2	THR	A	65	18.644	38.331	41.395	1.00	11.42	A
ATOM	478	C	THR	A	65	15.009	37.751	40.239	1.00	13.06	A
ATOM	479	O	THR	A	65	14.530	38.268	39.233	1.00	9.78	A
ATOM	480	N	ALA	A	66	14.272	37.374	41.281	1.00	11.93	A
ATOM	481	CA	ALA	A	66	12.831	37.607	41.287	1.00	16.82	A
ATOM	482	CB	ALA	A	66	12.231	37.106	42.601	1.00	17.23	A
ATOM	483	C	ALA	A	66	12.527	39.104	41.105	1.00	14.69	A
ATOM	484	O	ALA	A	66	11.587	39.467	40.409	1.00	12.67	A
ATOM	485	N	SER	A	67	13.322	39.962	41.744	1.00	15.98	A
ATOM	486	CA	SER	A	67	13.150	41.417	41.640	1.00	12.48	A
ATOM	487	CB	SER	A	67	14.108	42.166	42.579	1.00	18.87	A
ATOM	488	OG	SER	A	67	13.662	42.081	43.921	1.00	28.18	A
ATOM	489	C	SER	A	67	13.403	41.890	40.212	1.00	12.05	A
ATOM	490	O	SER	A	67	12.630	42.671	39.666	1.00	12.31	A
ATOM	491	N	GLN	A	68	14.495	41.426	39.616	1.00	8.93	A
ATOM	492	CA	GLN	A	68	14.796	41.803	38.237	1.00	8.58	A
ATOM	493	CB	GLN	A	68	16.123	41.176	37.768	1.00	11.33	A
ATOM	494	CG	GLN	A	68	17.343	41.749	38.524	1.00	12.20	A
ATOM	495	CD	GLN	A	68	18.656	41.026	38.242	1.00	15.53	A
ATOM	496	OE1	GLN	A	68	18.690	39.815	38.034	1.00	11.56	A
ATOM	497	NE2	GLN	A	68	19.743	41.770	38.255	1.00	14.33	A
ATOM	498	C	GLN	A	68	13.673	41.385	37.290	1.00	12.61	A
ATOM	499	O	GLN	A	68	13.270	42.158	36.423	1.00	10.84	A
ATOM	500	N	LEU	A	69	13.163	40.164	37.455	1.00	13.81	A
ATOM	501	CA	LEU	A	69	12.093	39.687	36.576	1.00	13.47	A
ATOM	502	CB	LEU	A	69	11.809	38.189	36.829	1.00	13.08	A
ATOM	503	CG	LEU	A	69	12.989	37.268	36.496	1.00	14.83	A
ATOM	504	CD1	LEU	A	69	12.772	35.862	37.071	1.00	16.18	A
ATOM	505	CD2	LEU	A	69	13.140	37.233	34.981	1.00	11.50	A
ATOM	506	C	LEU	A	69	10.810	40.484	36.778	1.00	13.14	A
ATOM	507	O	LEU	A	69	10.138	40.860	35.814	1.00	13.07	A
ATOM	508	N	ALA	A	70	10.465	40.728	38.034	1.00	12.61	A
ATOM	509	CA	ALA	A	70	9.227	41.443	38.328	1.00	12.01	A
ATOM	510	CB	ALA	A	70	8.951	41.453	39.841	1.00	13.19	A
ATOM	511	C	ALA	A	70	9.275	42.852	37.785	1.00	12.44	A
ATOM	512	O	ALA	A	70	8.297	43.334	37.240	1.00	16.48	A
ATOM	513	N	THR	A	71	10.419	43.512	37.928	1.00	12.49	A
ATOM	514	CA	THR	A	71	10.574	44.865	37.436	1.00	11.47	A
ATOM	515	CB	THR	A	71	11.914	45.463	37.941	1.00	18.09	A
ATOM	516	OG1	THR	A	71	11.834	45.621	39.370	1.00	19.27	A
ATOM	517	CG2	THR	A	71	12.225	46.811	37.267	1.00	13.43	A
ATOM	518	C	THR	A	71	10.501	44.905	35.902	1.00	11.57	A
ATOM	519	O	THR	A	71	9.881	45.800	35.337	1.00	15.24	A
ATOM	520	N	TYR	A	72	11.116	43.941	35.223	1.00	13.13	A
ATOM	521	CA	TYR	A	72	11.049	43.941	33.760	1.00	12.95	A
ATOM	522	CB	TYR	A	72	11.927	42.839	33.174	1.00	11.21	A
ATOM	523	CG	TYR	A	72	12.194	43.011	31.682	1.00	12.14	A
ATOM	524	CD1	TYR	A	72	13.122	43.936	31.224	1.00	11.17	A
ATOM	525	CE1	TYR	A	72	13.376	44.101	29.841	1.00	11.35	A
ATOM	526	CD2	TYR	A	72	11.515	42.239	30.736	1.00	14.03	A
ATOM	527	CE2	TYR	A	72	11.765	42.378	29.372	1.00	8.40	A

FIGURE 5 (continued)

12 / 46

ATOM	528	CZ	TYR	A	72	12.689	43.303	28.928	1.00	10.19	A
ATOM	529	OH	TYR	A	72	12.949	43.425	27.585	1.00	10.75	A
ATOM	530	C	TYR	A	72	9.604	43.705	33.313	1.00	13.42	A
ATOM	531	O	TYR	A	72	9.111	44.346	32.394	1.00	14.74	A
ATOM	532	N	ALA	A	73	8.943	42.763	33.970	1.00	14.68	A
ATOM	533	CA	ALA	A	73	7.563	42.423	33.650	1.00	15.37	A
ATOM	534	CB	ALA	A	73	7.090	41.293	34.556	1.00	10.74	A
ATOM	535	C	ALA	A	73	6.631	43.626	33.791	1.00	14.04	A
ATOM	536	O	ALA	A	73	5.711	43.811	32.992	1.00	13.32	A
ATOM	537	N	ALA	A	74	6.856	44.436	34.815	1.00	16.88	A
ATOM	538	CA	ALA	A	74	6.006	45.602	35.032	1.00	17.08	A
ATOM	539	CB	ALA	A	74	6.082	46.052	36.505	1.00	13.94	A
ATOM	540	C	ALA	A	74	6.354	46.768	34.118	1.00	20.94	A
ATOM	541	O	ALA	A	74	5.475	47.357	33.476	1.00	17.04	A
ATOM	542	N	ASN	A	75	7.645	47.061	34.014	1.00	15.74	A
ATOM	543	CA	ASN	A	75	8.125	48.203	33.241	1.00	17.76	A
ATOM	544	CB	ASN	A	75	9.439	48.712	33.839	1.00	19.52	A
ATOM	545	CG	ASN	A	75	9.308	49.152	35.289	1.00	24.86	A
ATOM	546	OD1	ASN	A	75	10.308	49.485	35.929	1.00	26.13	A
ATOM	547	ND2	ASN	A	75	8.084	49.150	35.816	1.00	27.41	A
ATOM	548	C	ASN	A	75	8.356	48.070	31.741	1.00	18.90	A
ATOM	549	O	ASN	A	75	8.049	48.996	30.986	1.00	16.37	A
ATOM	550	N	LYS	A	76	8.910	46.944	31.304	1.00	13.20	A
ATOM	551	CA	LYS	A	76	9.235	46.810	29.888	1.00	14.05	A
ATOM	552	CB	LYS	A	76	10.709	46.412	29.730	1.00	11.81	A
ATOM	553	CG	LYS	A	76	11.706	47.189	30.561	1.00	15.12	A
ATOM	554	CD	LYS	A	76	11.710	48.673	30.208	1.00	18.17	A
ATOM	555	CE	LYS	A	76	12.942	49.342	30.783	1.00	21.75	A
ATOM	556	NZ	LYS	A	76	12.858	50.832	30.665	1.00	23.76	A
ATOM	557	C	LYS	A	76	8.414	45.835	29.064	1.00	14.89	A
ATOM	558	O	LYS	A	76	8.184	46.053	27.874	1.00	15.18	A
ATOM	559	N	GLN	A	77	7.996	44.746	29.686	1.00	13.65	A
ATOM	560	CA	GLN	A	77	7.240	43.718	28.978	1.00	15.70	A
ATOM	561	CB	GLN	A	77	6.865	42.625	29.964	1.00	14.98	A
ATOM	562	CG	GLN	A	77	6.139	41.438	29.381	1.00	18.91	A
ATOM	563	CD	GLN	A	77	5.848	40.392	30.441	1.00	26.71	A
ATOM	564	OE1	GLN	A	77	6.747	39.965	31.167	1.00	25.14	A
ATOM	565	NE2	GLN	A	77	4.593	39.968	30.534	1.00	21.79	A
ATOM	566	C	GLN	A	77	5.989	44.205	28.222	1.00	16.81	A
ATOM	567	O	GLN	A	77	5.718	43.746	27.114	1.00	17.54	A
ATOM	568	N	PRO	A	78	5.216	45.142	28.800	1.00	19.48	A
ATOM	569	CD	PRO	A	78	5.255	45.765	30.134	1.00	12.68	A
ATOM	570	CA	PRO	A	78	4.023	45.575	28.056	1.00	15.54	A
ATOM	571	CB	PRO	A	78	3.428	46.654	28.958	1.00	19.25	A
ATOM	572	CG	PRO	A	78	3.787	46.150	30.342	1.00	17.82	A
ATOM	573	C	PRO	A	78	4.325	46.080	26.646	1.00	20.10	A
ATOM	574	O	PRO	A	78	3.614	45.748	25.692	1.00	18.30	A
ATOM	575	N	GLY	A	79	5.393	46.860	26.512	1.00	15.27	A
ATOM	576	CA	GLY	A	79	5.745	47.379	25.210	1.00	17.02	A
ATOM	577	C	GLY	A	79	6.802	46.616	24.427	1.00	20.02	A
ATOM	578	O	GLY	A	79	6.839	46.731	23.199	1.00	15.38	A
ATOM	579	N	TRP	A	80	7.639	45.830	25.111	1.00	13.75	A
ATOM	580	CA	TRP	A	80	8.723	45.092	24.440	1.00	14.43	A
ATOM	581	CB	TRP	A	80	10.062	45.359	25.136	1.00	11.39	A
ATOM	582	CG	TRP	A	80	10.549	46.780	25.071	1.00	15.13	A
ATOM	583	CD2	TRP	A	80	11.672	47.329	25.767	1.00	13.37	A
ATOM	584	CE2	TRP	A	80	11.823	48.666	25.332	1.00	13.52	A
ATOM	585	CE3	TRP	A	80	12.573	46.817	26.716	1.00	12.51	A
ATOM	586	CD1	TRP	A	80	10.068	47.779	24.271	1.00	19.04	A
ATOM	587	NE1	TRP	A	80	10.831	48.919	24.418	1.00	16.58	A
ATOM	588	CZ2	TRP	A	80	12.840	49.502	25.812	1.00	15.28	A
ATOM	589	CZ3	TRP	A	80	13.586	47.645	27.197	1.00	13.05	A
ATOM	590	CH2	TRP	A	80	13.710	48.979	26.739	1.00	16.82	A
ATOM	591	C	TRP	A	80	8.560	43.580	24.349	1.00	16.83	A
ATOM	592	O	TRP	A	80	9.361	42.909	23.685	1.00	16.92	A
ATOM	593	N	GLY	A	81	7.562	43.031	25.033	1.00	15.56	A
ATOM	594	CA	GLY	A	81	7.380	41.584	25.001	1.00	11.72	A
ATOM	595	C	GLY	A	81	8.071	40.921	26.186	1.00	13.05	A
ATOM	596	O	GLY	A	81	8.856	41.557	26.894	1.00	8.85	A
ATOM	597	N	LYS	A	82	7.784	39.638	26.395	1.00	10.46	A
ATOM	598	CA	LYS	A	82	8.374	38.882	27.499	1.00	11.96	A
ATOM	599	CB	LYS	A	82	7.702	37.506	27.608	1.00	11.82	A
ATOM	600	CG	LYS	A	82	6.341	37.497	28.315	1.00	12.27	A
ATOM	601	CD	LYS	A	82	5.578	36.167	28.137	1.00	15.83	A
ATOM	602	CE	LYS	A	82	6.296	34.971	28.782	1.00	21.44	A
ATOM	603	NZ	LYS	A	82	6.571	35.179	30.234	1.00	18.30	A

FIGURE 5 (continued)

13 / 46

ATOM	604	C	LYS	A	82	9.868	38.658	27.275	1.00	12.45	A
ATOM	605	O	LYS	A	82	10.313	38.530	26.126	1.00	11.99	A
ATOM	606	N	LEU	A	83	10.649	38.598	28.357	1.00	10.87	A
ATOM	607	CA	LEU	A	83	12.057	38.305	28.161	1.00	10.47	A
ATOM	608	CB	LEU	A	83	12.955	38.929	29.248	1.00	16.59	A
ATOM	609	CG	LEU	A	83	13.059	38.501	30.707	1.00	13.98	A
ATOM	610	CD1	LEU	A	83	13.627	37.083	30.856	1.00	13.97	A
ATOM	611	CD2	LEU	A	83	14.010	39.508	31.412	1.00	12.95	A
ATOM	612	C	LEU	A	83	12.191	36.790	28.142	1.00	8.84	A
ATOM	613	O	LEU	A	83	11.288	36.062	28.604	1.00	12.14	A
ATOM	614	N	ILE	A	84	13.294	36.330	27.567	1.00	9.04	A
ATOM	615	CA	ILE	A	84	13.606	34.912	27.467	1.00	7.94	A
ATOM	616	CB	ILE	A	84	13.734	34.492	25.986	1.00	11.27	A
ATOM	617	CG2	ILE	A	84	14.322	33.075	25.875	1.00	15.02	A
ATOM	618	CG1	ILE	A	84	12.356	34.567	25.306	1.00	13.46	A
ATOM	619	CD1	ILE	A	84	12.407	34.310	23.806	1.00	10.66	A
ATOM	620	C	ILE	A	84	14.957	34.682	28.151	1.00	9.44	A
ATOM	621	O	ILE	A	84	15.918	35.410	27.891	1.00	9.33	A
ATOM	622	N	GLU	A	85	15.018	33.686	29.023	1.00	7.70	A
ATOM	623	CA	GLU	A	85	16.269	33.331	29.683	1.00	8.79	A
ATOM	624	CB	GLU	A	85	16.211	33.631	31.196	1.00	7.98	A
ATOM	625	CG	GLU	A	85	17.532	33.291	31.922	1.00	8.35	A
ATOM	626	CD	GLU	A	85	17.472	33.466	33.442	1.00	9.44	A
ATOM	627	OE1	GLU	A	85	16.520	32.969	34.103	1.00	13.35	A
ATOM	628	OE2	GLU	A	85	18.408	34.077	33.998	1.00	10.18	A
ATOM	629	C	GLU	A	85	16.452	31.832	29.442	1.00	9.15	A
ATOM	630	O	GLU	A	85	15.614	31.047	29.870	1.00	10.73	A
ATOM	631	N	VAL	A	86	17.513	31.438	28.733	1.00	9.15	A
ATOM	632	CA	VAL	A	86	17.772	30.021	28.458	1.00	9.61	A
ATOM	633	CB	VAL	A	86	17.394	29.631	26.987	1.00	8.48	A
ATOM	634	CG1	VAL	A	86	15.866	29.641	26.795	1.00	11.82	A
ATOM	635	CG2	VAL	A	86	18.062	30.587	25.998	1.00	8.25	A
ATOM	636	C	VAL	A	86	19.247	29.653	28.653	1.00	12.36	A
ATOM	637	O	VAL	A	86	20.135	30.490	28.488	1.00	7.65	A
ATOM	638	N	PRO	A	87	19.530	28.392	29.034	1.00	7.50	A
ATOM	639	CD	PRO	A	87	18.611	27.261	29.245	1.00	11.19	A
ATOM	640	CA	PRO	A	87	20.927	27.986	29.213	1.00	8.03	A
ATOM	641	CB	PRO	A	87	20.806	26.551	29.747	1.00	11.47	A
ATOM	642	CG	PRO	A	87	19.531	26.065	29.123	1.00	18.08	A
ATOM	643	C	PRO	A	87	21.551	28.031	27.803	1.00	12.05	A
ATOM	644	O	PRO	A	87	20.845	27.799	26.798	1.00	11.64	A
ATOM	645	N	SER	A	88	22.844	28.346	27.739	1.00	10.05	A
ATOM	646	CA	SER	A	88	23.607	28.427	26.480	1.00	8.91	A
ATOM	647	CB	SER	A	88	24.472	29.695	26.471	1.00	6.92	A
ATOM	648	OG	SER	A	88	25.266	29.787	25.294	1.00	11.36	A
ATOM	649	C	SER	A	88	24.484	27.177	26.379	1.00	7.85	A
ATOM	650	O	SER	A	88	24.385	26.432	25.401	1.00	7.71	A
ATOM	651	N	VAL	A	89	25.365	26.993	27.368	1.00	7.73	A
ATOM	652	CA	VAL	A	89	26.218	25.802	27.481	1.00	8.66	A
ATOM	653	CB	VAL	A	89	27.639	26.010	26.874	1.00	5.11	A
ATOM	654	CG1	VAL	A	89	27.522	26.503	25.400	1.00	7.72	A
ATOM	655	CG2	VAL	A	89	28.444	27.016	27.744	1.00	8.02	A
ATOM	656	C	VAL	A	89	26.407	25.527	28.980	1.00	10.90	A
ATOM	657	O	VAL	A	89	26.037	26.356	29.809	1.00	9.82	A
ATOM	658	N	ALA	A	90	26.982	24.369	29.325	1.00	10.64	A
ATOM	659	CA	ALA	A	90	27.242	24.059	30.722	1.00	8.29	A
ATOM	660	CB	ALA	A	90	26.792	22.616	31.077	1.00	8.16	A
ATOM	661	C	ALA	A	90	28.764	24.190	30.863	1.00	7.63	A
ATOM	662	O	ALA	A	90	29.498	24.095	29.880	1.00	7.66	A
ATOM	663	N	THR	A	91	29.233	24.345	32.091	1.00	7.77	A
ATOM	664	CA	THR	A	91	30.651	24.559	32.300	1.00	9.18	A
ATOM	665	CB	THR	A	91	30.945	26.074	32.165	1.00	10.09	A
ATOM	666	OG1	THR	A	91	32.337	26.323	32.365	1.00	11.79	A
ATOM	667	CG2	THR	A	91	30.156	26.862	33.214	1.00	11.41	A
ATOM	668	C	THR	A	91	31.116	24.140	33.686	1.00	10.91	A
ATOM	669	O	THR	A	91	30.326	24.055	34.614	1.00	9.96	A
ATOM	670	N	SER	A	92	32.409	23.858	33.811	1.00	11.52	A
ATOM	671	CA	SER	A	92	32.972	23.598	35.122	1.00	9.75	A
ATOM	672	CB	SER	A	92	34.167	22.642	35.011	1.00	12.03	A
ATOM	673	OG	SER	A	92	35.213	23.181	34.186	1.00	10.62	A
ATOM	674	C	SER	A	92	33.490	24.962	35.601	1.00	10.73	A
ATOM	675	O	SER	A	92	33.397	25.974	34.883	1.00	8.53	A
ATOM	676	N	VAL	A	93	33.980	25.003	36.837	1.00	8.68	A
ATOM	677	CA	VAL	A	93	34.640	26.197	37.369	1.00	7.08	A
ATOM	678	CB	VAL	A	93	34.010	26.736	38.667	1.00	7.09	A
ATOM	679	CG1	VAL	A	93	34.896	27.906	39.215	1.00	10.40	A

FIGURE 5 (continued)

14 / 46

ATOM	680	CG2	VAL	A	93	32.592	27.269	38.376	1.00	10.45	A
ATOM	681	C	VAL	A	93	36.033	25.643	37.694	1.00	9.49	A
ATOM	682	O	VAL	A	93	36.162	24.745	38.527	1.00	12.26	A
ATOM	683	N	ALA	A	94	37.064	26.148	37.025	1.00	8.00	A
ATOM	684	CA	ALA	A	94	38.425	25.645	37.236	1.00	8.64	A
ATOM	685	CB	ALA	A	94	39.204	25.722	35.921	1.00	7.88	A
ATOM	686	C	ALA	A	94	39.197	26.374	38.329	1.00	7.97	A
ATOM	687	O	ALA	A	94	38.906	27.530	38.625	1.00	8.61	A
ATOM	688	N	ILE	A	95	40.210	25.709	38.894	1.00	5.77	A
ATOM	689	CA	ILE	A	95	41.016	26.290	39.963	1.00	7.30	A
ATOM	690	CB	ILE	A	95	40.870	25.486	41.307	1.00	9.66	A
ATOM	691	CG2	ILE	A	95	41.522	26.261	42.465	1.00	6.29	A
ATOM	692	CG1	ILE	A	95	39.401	25.218	41.641	1.00	10.13	A
ATOM	693	CD1	ILE	A	95	38.566	26.491	41.909	1.00	13.60	A
ATOM	694	C	ILE	A	95	42.496	26.263	39.572	1.00	8.10	A
ATOM	695	O	ILE	A	95	43.261	25.373	40.001	1.00	10.23	A
ATOM	696	N	PRO	A	96	42.923	27.216	38.742	1.00	6.65	A
ATOM	697	CD	PRO	A	96	42.133	28.263	38.063	1.00	6.16	A
ATOM	698	CA	PRO	A	96	44.330	27.265	38.326	1.00	7.43	A
ATOM	699	CB	PRO	A	96	44.275	28.107	37.054	1.00	9.06	A
ATOM	700	CG	PRO	A	96	43.207	29.147	37.446	1.00	8.84	A
ATOM	701	C	PRO	A	96	45.133	27.938	39.434	1.00	10.94	A
ATOM	702	O	PRO	A	96	44.574	28.645	40.277	1.00	8.21	A
ATOM	703	N	PHE	A	97	46.441	27.715	39.447	1.00	9.05	A
ATOM	704	CA	PHE	A	97	47.276	28.302	40.480	1.00	8.97	A
ATOM	705	CB	PHE	A	97	47.259	27.414	41.732	1.00	10.70	A
ATOM	706	CG	PHE	A	97	47.748	26.015	41.477	1.00	9.86	A
ATOM	707	CD1	PHE	A	97	49.114	25.720	41.524	1.00	10.13	A
ATOM	708	CD2	PHE	A	97	46.862	25.010	41.121	1.00	7.97	A
ATOM	709	CE1	PHE	A	97	49.589	24.436	41.211	1.00	9.97	A
ATOM	710	CE2	PHE	A	97	47.326	23.704	40.802	1.00	8.94	A
ATOM	711	CZ	PHE	A	97	48.709	23.433	40.852	1.00	7.63	A
ATOM	712	C	PHE	A	97	48.698	28.418	39.949	1.00	9.55	A
ATOM	713	O	PHE	A	97	49.054	27.761	38.962	1.00	9.51	A
ATOM	714	N	ARG	A	98	49.498	29.260	40.597	1.00	8.26	A
ATOM	715	CA	ARG	A	98	50.900	29.457	40.205	1.00	11.26	A
ATOM	716	CB	ARG	A	98	51.149	30.927	39.808	1.00	13.41	A
ATOM	717	CG	ARG	A	98	52.624	31.218	39.452	1.00	12.41	A
ATOM	718	CD	ARG	A	98	52.902	32.648	39.002	1.00	15.00	A
ATOM	719	NE	ARG	A	98	54.350	32.871	38.907	1.00	20.95	A
ATOM	720	CZ	ARG	A	98	55.048	33.714	39.670	1.00	19.61	A
ATOM	721	NH1	ARG	A	98	54.454	34.446	40.606	1.00	16.05	A
ATOM	722	NH2	ARG	A	98	56.361	33.824	39.500	1.00	22.95	A
ATOM	723	C	ARG	A	98	51.765	29.079	41.415	1.00	9.82	A
ATOM	724	O	ARG	A	98	51.955	29.881	42.327	1.00	12.72	A
ATOM	725	N	LYS	A	99	52.258	27.838	41.417	1.00	13.72	A
ATOM	726	CA	LYS	A	99	53.081	27.314	42.510	1.00	14.88	A
ATOM	727	CB	LYS	A	99	52.179	26.922	43.688	1.00	10.80	A
ATOM	728	CG	LYS	A	99	52.899	26.401	44.919	1.00	8.32	A
ATOM	729	CD	LYS	A	99	53.744	27.518	45.557	1.00	10.62	A
ATOM	730	CE	LYS	A	99	54.525	27.007	46.790	1.00	10.76	A
ATOM	731	NZ	LYS	A	99	55.346	28.125	47.368	1.00	13.56	A
ATOM	732	C	LYS	A	99	53.809	26.095	41.956	1.00	14.43	A
ATOM	733	O	LYS	A	99	53.200	25.056	41.701	1.00	15.34	A
ATOM	734	N	ALA	A	100	55.120	26.226	41.769	1.00	12.67	A
ATOM	735	CA	ALA	A	100	55.911	25.143	41.202	1.00	14.53	A
ATOM	736	CB	ALA	A	100	57.354	25.629	40.914	1.00	14.12	A
ATOM	737	C	ALA	A	100	55.960	23.900	42.072	1.00	14.42	A
ATOM	738	O	ALA	A	100	55.929	23.987	43.303	1.00	16.53	A
ATOM	739	N	GLY	A	101	56.061	22.751	41.409	1.00	10.16	A
ATOM	740	CA	GLY	A	101	56.133	21.476	42.096	1.00	11.78	A
ATOM	741	C	GLY	A	101	55.786	20.360	41.136	1.00	17.78	A
ATOM	742	O	GLY	A	101	54.853	20.479	40.338	1.00	14.78	A
ATOM	743	N	GLY	A	102	56.543	19.274	41.195	1.00	13.81	A
ATOM	744	CA	GLY	A	102	56.273	18.156	40.313	1.00	20.81	A
ATOM	745	C	GLY	A	102	55.051	17.348	40.720	1.00	16.58	A
ATOM	746	O	GLY	A	102	54.498	16.627	39.898	1.00	16.24	A
ATOM	747	N	ASN	A	103	54.624	17.451	41.976	1.00	17.72	A
ATOM	748	CA	ASN	A	103	53.465	16.675	42.434	1.00	16.85	A
ATOM	749	CB	ASN	A	103	53.372	16.694	43.963	1.00	15.22	A
ATOM	750	CG	ASN	A	103	54.365	15.760	44.615	1.00	23.02	A
ATOM	751	OD1	ASN	A	103	55.279	15.249	43.955	1.00	19.32	A
ATOM	752	ND2	ASN	A	103	54.205	15.535	45.916	1.00	15.75	A
ATOM	753	C	ASN	A	103	52.145	17.197	41.885	1.00	15.38	A
ATOM	754	O	ASN	A	103	51.991	18.390	41.666	1.00	11.02	A
ATOM	755	N	ALA	A	104	51.183	16.306	41.693	1.00	16.02	A

FIGURE 5 (continued)

15 / 46

ATOM	756	CA	ALA	A	104	49.880	16.744	41.219	1.00	16.65	A
ATOM	757	CB	ALA	A	104	49.068	15.538	40.741	1.00	20.27	A
ATOM	758	C	ALA	A	104	49.170	17.427	42.395	1.00	15.98	A
ATOM	759	O	ALA	A	104	49.298	16.986	43.531	1.00	15.25	A
ATOM	760	N	VAL	A	105	48.470	18.530	42.127	1.00	13.62	A
ATOM	761	CA	VAL	A	105	47.701	19.227	43.157	1.00	13.77	A
ATOM	762	CB	VAL	A	105	47.708	20.756	42.945	1.00	15.80	A
ATOM	763	CG1	VAL	A	105	46.645	21.409	43.814	1.00	16.24	A
ATOM	764	CG2	VAL	A	105	49.081	21.310	43.295	1.00	15.48	A
ATOM	765	C	VAL	A	105	46.273	18.699	43.026	1.00	13.93	A
ATOM	766	O	VAL	A	105	45.634	18.867	41.982	1.00	11.00	A
ATOM	767	N	ASP	A	106	45.781	18.059	44.085	1.00	11.30	A
ATOM	768	CA	ASP	A	106	44.446	17.447	44.087	1.00	13.33	A
ATOM	769	CB	ASP	A	106	44.594	15.914	44.007	1.00	15.23	A
ATOM	770	CG	ASP	A	106	43.266	15.181	43.763	1.00	18.75	A
ATOM	771	OD1	ASP	A	106	43.294	13.932	43.636	1.00	20.08	A
ATOM	772	OD2	ASP	A	106	42.201	15.832	43.705	1.00	16.37	A
ATOM	773	C	ASP	A	106	43.748	17.854	45.371	1.00	13.44	A
ATOM	774	O	ASP	A	106	44.013	17.312	46.441	1.00	12.47	A
ATOM	775	N	LEU	A	107	42.838	18.809	45.256	1.00	12.47	A
ATOM	776	CA	LEU	A	107	42.126	19.322	46.424	1.00	10.60	A
ATOM	777	CB	LEU	A	107	41.608	20.743	46.139	1.00	9.94	A
ATOM	778	CG	LEU	A	107	42.656	21.830	45.874	1.00	15.11	A
ATOM	779	CD1	LEU	A	107	41.992	23.049	45.233	1.00	12.77	A
ATOM	780	CD2	LEU	A	107	43.332	22.222	47.191	1.00	15.50	A
ATOM	781	C	LEU	A	107	40.936	18.504	46.860	1.00	11.58	A
ATOM	782	O	LEU	A	107	40.118	18.134	46.029	1.00	11.26	A
ATOM	783	N	SER	A	108	40.840	18.205	48.157	1.00	10.03	A
ATOM	784	CA	SER	A	108	39.632	17.555	48.632	1.00	9.49	A
ATOM	785	CB	SER	A	108	39.823	16.938	50.026	1.00	11.45	A
ATOM	786	OG	SER	A	108	40.112	17.944	50.988	1.00	10.62	A
ATOM	787	C	SER	A	108	38.686	18.762	48.734	1.00	13.88	A
ATOM	788	O	SER	A	108	39.137	19.909	48.733	1.00	9.31	A
ATOM	789	N	VAL	A	109	37.384	18.528	48.795	1.00	11.62	A
ATOM	790	CA	VAL	A	109	36.456	19.648	48.915	1.00	12.52	A
ATOM	791	CB	VAL	A	109	34.997	19.149	48.822	1.00	14.25	A
ATOM	792	CG1	VAL	A	109	34.022	20.273	49.172	1.00	10.43	A
ATOM	793	CG2	VAL	A	109	34.738	18.624	47.385	1.00	9.95	A
ATOM	794	C	VAL	A	109	36.705	20.397	50.228	1.00	8.60	A
ATOM	795	O	VAL	A	109	36.646	21.622	50.265	1.00	9.21	A
ATOM	796	N	LYS	A	110	36.995	19.666	51.301	1.00	9.28	A
ATOM	797	CA	LYS	A	110	37.307	20.306	52.593	1.00	7.04	A
ATOM	798	CB	LYS	A	110	37.597	19.237	53.650	1.00	7.60	A
ATOM	799	CG	LYS	A	110	38.038	19.793	55.030	1.00	9.51	A
ATOM	800	CD	LYS	A	110	36.987	20.726	55.655	1.00	7.71	A
ATOM	801	CE	LYS	A	110	37.436	21.170	57.033	1.00	15.09	A
ATOM	802	NZ	LYS	A	110	36.482	22.129	57.688	1.00	11.10	A
ATOM	803	C	LYS	A	110	38.532	21.234	52.452	1.00	8.55	A
ATOM	804	O	LYS	A	110	38.588	22.313	53.040	1.00	9.65	A
ATOM	805	N	GLU	A	111	39.530	20.803	51.696	1.00	8.56	A
ATOM	806	CA	GLU	A	111	40.711	21.640	51.495	1.00	11.39	A
ATOM	807	CB	GLU	A	111	41.817	20.836	50.800	1.00	13.45	A
ATOM	808	CG	GLU	A	111	42.582	19.940	51.784	1.00	15.25	A
ATOM	809	CD	GLU	A	111	43.527	18.960	51.098	1.00	16.99	A
ATOM	810	OE1	GLU	A	111	44.310	18.296	51.808	1.00	12.70	A
ATOM	811	OE2	GLU	A	111	43.477	18.851	49.860	1.00	13.80	A
ATOM	812	C	GLU	A	111	40.342	22.881	50.663	1.00	12.16	A
ATOM	813	O	GLU	A	111	40.751	23.998	50.983	1.00	8.45	A
ATOM	814	N	LEU	A	112	39.586	22.680	49.587	1.00	11.50	A
ATOM	815	CA	LEU	A	112	39.157	23.802	48.753	1.00	11.60	A
ATOM	816	CB	LEU	A	112	38.127	23.339	47.728	1.00	12.29	A
ATOM	817	CG	LEU	A	112	37.520	24.486	46.906	1.00	13.68	A
ATOM	818	CD1	LEU	A	112	38.486	24.835	45.793	1.00	14.87	A
ATOM	819	CD2	LEU	A	112	36.183	24.067	46.307	1.00	23.81	A
ATOM	820	C	LEU	A	112	38.491	24.845	49.648	1.00	11.64	A
ATOM	821	O	LEU	A	112	38.782	26.036	49.569	1.00	9.35	A
ATOM	822	N	CYS	A	113	37.598	24.370	50.511	1.00	9.13	A
ATOM	823	CA	CYS	A	113	36.869	25.251	51.407	1.00	10.02	A
ATOM	824	C	CYS	A	113	37.806	26.040	52.332	1.00	10.42	A
ATOM	825	O	CYS	A	113	37.620	27.243	52.550	1.00	9.94	A
ATOM	826	CB	CYS	A	113	35.881	24.414	52.215	1.00	7.06	A
ATOM	827	SG	CYS	A	113	34.495	23.714	51.225	1.00	12.97	A
ATOM	828	N	GLY	A	114	38.815	25.357	52.854	1.00	8.53	A
ATOM	829	CA	GLY	A	114	39.774	25.979	53.746	1.00	8.15	A
ATOM	830	C	GLY	A	114	40.615	27.023	53.048	1.00	8.58	A
ATOM	831	O	GLY	A	114	40.974	28.045	53.660	1.00	9.42	A

FIGURE 5 (continued)

TITLE: NOVEL PHOSPHATE-BINDING PROTEIN, PHARMACEUTICAL COMPOSITIONS CONTAINING SAME AND USE THEREOF

16 / 46

ATOM	832	N	VAL	A	115	40.929	26.780	51.773	1.00	8.91	A
ATOM	833	CA	VAL	A	115	41.724	27.727	51.001	1.00	11.99	A
ATOM	834	CB	VAL	A	115	42.142	27.154	49.611	1.00	10.97	A
ATOM	835	CG1	VAL	A	115	42.754	28.274	48.736	1.00	12.08	A
ATOM	836	CG2	VAL	A	115	43.175	26.034	49.794	1.00	9.96	A
ATOM	837	C	VAL	A	115	40.933	28.999	50.769	1.00	10.50	A
ATOM	838	O	VAL	A	115	41.450	30.107	50.958	1.00	10.53	A
ATOM	839	N	PHE	A	116	39.672	28.856	50.383	1.00	10.04	A
ATOM	840	CA	PHE	A	116	38.885	30.046	50.123	1.00	12.53	A
ATOM	841	CB	PHE	A	116	37.891	29.774	49.000	1.00	8.51	A
ATOM	842	CG	PHE	A	116	38.564	29.656	47.664	1.00	8.77	A
ATOM	843	CD1	PHE	A	116	39.041	28.429	47.220	1.00	7.52	A
ATOM	844	CD2	PHE	A	116	38.792	30.791	46.892	1.00	10.79	A
ATOM	845	CE1	PHE	A	116	39.742	28.319	46.019	1.00	11.26	A
ATOM	846	CE2	PHE	A	116	39.494	30.708	45.682	1.00	12.98	A
ATOM	847	CZ	PHE	A	116	39.971	29.463	45.244	1.00	12.19	A
ATOM	848	C	PHE	A	116	38.236	30.713	51.319	1.00	11.72	A
ATOM	849	O	PHE	A	116	37.688	31.802	51.180	1.00	10.01	A
ATOM	850	N	SER	A	117	38.323	30.077	52.493	1.00	7.36	A
ATOM	851	CA	SER	A	117	37.802	30.669	53.722	1.00	12.12	A
ATOM	852	CB	SER	A	117	37.217	29.605	54.654	1.00	11.41	A
ATOM	853	OG	SER	A	117	38.251	28.827	55.231	1.00	12.73	A
ATOM	854	C	SER	A	117	38.935	31.372	54.474	1.00	12.93	A
ATOM	855	O	SER	A	117	38.693	32.241	55.316	1.00	9.90	A
ATOM	856	N	GLY	A	118	40.169	30.988	54.174	1.00	14.10	A
ATOM	857	CA	GLY	A	118	41.312	31.576	54.860	1.00	13.07	A
ATOM	858	C	GLY	A	118	41.850	30.640	55.931	1.00	15.32	A
ATOM	859	O	GLY	A	118	42.935	30.873	56.484	1.00	15.65	A
ATOM	860	N	ARG	A	119	41.107	29.575	56.241	1.00	15.32	A
ATOM	861	CA	ARG	A	119	41.550	28.622	57.266	1.00	15.10	A
ATOM	862	CB	ARG	A	119	40.503	27.518	57.485	1.00	17.52	A
ATOM	863	CG	ARG	A	119	40.986	26.359	58.390	1.00	19.04	A
ATOM	864	CD	ARG	A	119	39.880	25.325	58.628	1.00	17.23	A
ATOM	865	NE	ARG	A	119	39.338	24.771	57.377	1.00	11.41	A
ATOM	866	CZ	ARG	A	119	39.828	23.717	56.727	1.00	13.77	A
ATOM	867	NH1	ARG	A	119	40.895	23.061	57.188	1.00	9.19	A
ATOM	868	NH2	ARG	A	119	39.239	23.317	55.607	1.00	10.56	A
ATOM	869	C	ARG	A	119	42.896	27.990	56.896	1.00	14.09	A
ATOM	870	O	ARG	A	119	43.749	27.784	57.757	1.00	12.49	A
ATOM	871	N	ILE	A	120	43.074	27.672	55.620	1.00	14.25	A
ATOM	872	CA	ILE	A	120	44.327	27.088	55.134	1.00	11.87	A
ATOM	873	CB	ILE	A	120	44.066	25.956	54.113	1.00	13.86	A
ATOM	874	CG2	ILE	A	120	45.373	25.443	53.529	1.00	12.88	A
ATOM	875	CG1	ILE	A	120	43.349	24.796	54.812	1.00	12.97	A
ATOM	876	CD1	ILE	A	120	42.920	23.638	53.863	1.00	12.93	A
ATOM	877	C	ILE	A	120	45.042	28.241	54.445	1.00	16.50	A
ATOM	878	O	ILE	A	120	44.606	28.704	53.391	1.00	15.43	A
ATOM	879	N	ALA	A	121	46.131	28.706	55.051	1.00	15.30	A
ATOM	880	CA	ALA	A	121	46.884	29.848	54.529	1.00	14.70	A
ATOM	881	CB	ALA	A	121	47.111	30.850	55.640	1.00	21.39	A
ATOM	882	C	ALA	A	121	48.211	29.482	53.904	1.00	15.45	A
ATOM	883	O	ALA	A	121	48.868	30.329	53.284	1.00	16.44	A
ATOM	884	N	ASN	A	122	48.608	28.227	54.056	1.00	12.07	A
ATOM	885	CA	ASN	A	122	49.887	27.789	53.507	1.00	12.53	A
ATOM	886	CB	ASN	A	122	50.853	27.467	54.660	1.00	13.64	A
ATOM	887	CG	ASN	A	122	52.279	27.293	54.188	1.00	16.68	A
ATOM	888	OD1	ASN	A	122	52.666	26.224	53.725	1.00	18.01	A
ATOM	889	ND2	ASN	A	122	53.063	28.363	54.279	1.00	14.68	A
ATOM	890	C	ASN	A	122	49.681	26.568	52.608	1.00	11.32	A
ATOM	891	O	ASN	A	122	48.809	25.737	52.865	1.00	11.94	A
ATOM	892	N	TRP	A	123	50.454	26.499	51.528	1.00	12.38	A
ATOM	893	CA	TRP	A	123	50.365	25.390	50.580	1.00	10.94	A
ATOM	894	CB	TRP	A	123	51.330	25.597	49.406	1.00	10.33	A
ATOM	895	CG	TRP	A	123	50.761	26.503	48.337	1.00	12.83	A
ATOM	896	CD2	TRP	A	123	49.900	26.108	47.261	1.00	10.58	A
ATOM	897	CE2	TRP	A	123	49.568	27.279	46.533	1.00	12.26	A
ATOM	898	CE3	TRP	A	123	49.381	24.884	46.841	1.00	12.52	A
ATOM	899	CD1	TRP	A	123	50.916	27.862	48.227	1.00	15.24	A
ATOM	900	NE1	TRP	A	123	50.198	28.334	47.140	1.00	12.70	A
ATOM	901	CZ2	TRP	A	123	48.732	27.256	45.403	1.00	10.92	A
ATOM	902	CZ3	TRP	A	123	48.547	24.863	45.710	1.00	16.36	A
ATOM	903	CH2	TRP	A	123	48.237	26.043	45.012	1.00	9.72	A
ATOM	904	C	TRP	A	123	50.661	24.045	51.213	1.00	13.55	A
ATOM	905	O	TRP	A	123	50.284	23.006	50.676	1.00	13.98	A
ATOM	906	N	SER	A	124	51.346	24.054	52.349	1.00	13.10	A
ATOM	907	CA	SER	A	124	51.654	22.801	53.010	1.00	11.36	A

FIGURE 5 (continued)

17 / 46

ATOM	908	CB	SER	A	124	52.670	23.038	54.135	1.00	11.89	A
ATOM	909	OG	SER	A	124	52.130	23.884	55.132	1.00	14.19	A
ATOM	910	C	SER	A	124	50.361	22.161	53.564	1.00	17.25	A
ATOM	911	O	SER	A	124	50.354	20.974	53.924	1.00	13.81	A
ATOM	912	N	GLY	A	125	49.273	22.937	53.617	1.00	13.73	A
ATOM	913	CA	GLY	A	125	47.999	22.416	54.117	1.00	13.26	A
ATOM	914	C	GLY	A	125	47.216	21.569	53.101	1.00	19.05	A
ATOM	915	O	GLY	A	125	46.116	21.066	53.404	1.00	15.82	A
ATOM	916	N	ILE	A	126	47.759	21.413	51.892	1.00	11.57	A
ATOM	917	CA	ILE	A	126	47.111	20.590	50.866	1.00	13.57	A
ATOM	918	CB	ILE	A	126	47.116	21.338	49.499	1.00	10.65	A
ATOM	919	CG2	ILE	A	126	46.584	20.440	48.369	1.00	10.73	A
ATOM	920	CG1	ILE	A	126	46.244	22.598	49.639	1.00	14.04	A
ATOM	921	CD1	ILE	A	126	46.355	23.571	48.474	1.00	21.47	A
ATOM	922	C	ILE	A	126	47.886	19.270	50.794	1.00	14.42	A
ATOM	923	O	ILE	A	126	49.012	19.228	50.299	1.00	12.48	A
ATOM	924	N	THR	A	127	47.287	18.199	51.310	1.00	14.33	A
ATOM	925	CA	THR	A	127	47.974	16.918	51.341	1.00	15.70	A
ATOM	926	CB	THR	A	127	47.144	15.848	52.079	1.00	20.78	A
ATOM	927	OG1	THR	A	127	45.978	15.519	51.309	1.00	21.71	A
ATOM	928	CG2	THR	A	127	46.719	16.379	53.462	1.00	19.06	A
ATOM	929	C	THR	A	127	48.389	16.389	49.978	1.00	15.85	A
ATOM	930	O	THR	A	127	47.628	16.442	49.011	1.00	15.48	A
ATOM	931	N	GLY	A	128	49.627	15.907	49.925	1.00	11.25	A
ATOM	932	CA	GLY	A	128	50.202	15.348	48.719	1.00	13.92	A
ATOM	933	C	GLY	A	128	50.726	16.299	47.655	1.00	15.93	A
ATOM	934	O	GLY	A	128	51.360	15.837	46.718	1.00	18.28	A
ATOM	935	N	ALA	A	129	50.491	17.610	47.788	1.00	13.36	A
ATOM	936	CA	ALA	A	129	50.929	18.558	46.765	1.00	14.53	A
ATOM	937	CB	ALA	A	129	50.138	19.873	46.886	1.00	13.51	A
ATOM	938	C	ALA	A	129	52.428	18.856	46.777	1.00	20.08	A
ATOM	939	O	ALA	A	129	52.954	19.427	45.811	1.00	13.92	A
ATOM	940	N	GLY	A	130	53.110	18.489	47.863	1.00	15.72	A
ATOM	941	CA	GLY	A	130	54.552	18.715	47.931	1.00	18.22	A
ATOM	942	C	GLY	A	130	54.937	20.167	47.720	1.00	17.01	A
ATOM	943	O	GLY	A	130	55.944	20.485	47.088	1.00	16.95	A
ATOM	944	N	ARG	A	131	54.130	21.059	48.274	1.00	14.88	A
ATOM	945	CA	ARG	A	131	54.361	22.500	48.142	1.00	14.67	A
ATOM	946	CB	ARG	A	131	53.312	23.102	47.190	1.00	10.65	A
ATOM	947	CG	ARG	A	131	53.506	22.713	45.730	1.00	14.78	A
ATOM	948	CD	ARG	A	131	52.234	22.985	44.895	1.00	13.27	A
ATOM	949	NE	ARG	A	131	52.479	22.959	43.441	1.00	13.40	A
ATOM	950	CZ	ARG	A	131	52.670	21.873	42.695	1.00	12.12	A
ATOM	951	NH1	ARG	A	131	52.880	22.010	41.383	1.00	12.83	A
ATOM	952	NH2	ARG	A	131	52.656	20.660	43.233	1.00	13.76	A
ATOM	953	C	ARG	A	131	54.217	23.171	49.502	1.00	14.12	A
ATOM	954	O	ARG	A	131	53.451	22.703	50.329	1.00	15.12	A
ATOM	955	N	SER	A	132	54.948	24.258	49.730	1.00	12.39	A
ATOM	956	CA	SER	A	132	54.830	24.987	50.990	1.00	15.94	A
ATOM	957	CB	SER	A	132	55.817	24.450	52.046	1.00	22.25	A
ATOM	958	OG	SER	A	132	57.143	24.690	51.644	1.00	25.99	A
ATOM	959	C	SER	A	132	55.070	26.468	50.735	1.00	12.92	A
ATOM	960	O	SER	A	132	55.695	26.857	49.746	1.00	16.84	A
ATOM	961	N	GLY	A	133	54.570	27.300	51.634	1.00	14.33	A
ATOM	962	CA	GLY	A	133	54.695	28.734	51.442	1.00	14.73	A
ATOM	963	C	GLY	A	133	53.295	29.318	51.394	1.00	14.56	A
ATOM	964	O	GLY	A	133	52.320	28.589	51.183	1.00	12.31	A
ATOM	965	N	PRO	A	134	53.162	30.633	51.561	1.00	15.09	A
ATOM	966	CD	PRO	A	134	54.254	31.607	51.743	1.00	16.35	A
ATOM	967	CA	PRO	A	134	51.854	31.291	51.548	1.00	14.55	A
ATOM	968	CB	PRO	A	134	52.196	32.760	51.828	1.00	20.54	A
ATOM	969	CG	PRO	A	134	53.623	32.900	51.266	1.00	21.58	A
ATOM	970	C	PRO	A	134	50.997	31.143	50.299	1.00	16.29	A
ATOM	971	O	PRO	A	134	51.509	31.105	49.180	1.00	12.69	A
ATOM	972	N	ILE	A	135	49.685	31.057	50.527	1.00	13.39	A
ATOM	973	CA	ILE	A	135	48.688	30.973	49.454	1.00	13.74	A
ATOM	974	CB	ILE	A	135	47.523	30.010	49.801	1.00	15.95	A
ATOM	975	CG2	ILE	A	135	46.417	30.115	48.727	1.00	13.97	A
ATOM	976	CG1	ILE	A	135	48.032	28.582	49.918	1.00	15.73	A
ATOM	977	CD1	ILE	A	135	46.988	27.607	50.453	1.00	15.61	A
ATOM	978	C	ILE	A	135	48.077	32.366	49.353	1.00	13.04	A
ATOM	979	O	ILE	A	135	47.757	32.983	50.372	1.00	15.69	A
ATOM	980	N	GLN	A	136	47.918	32.872	48.136	1.00	11.91	A
ATOM	981	CA	GLN	A	136	47.319	34.190	47.958	1.00	11.20	A
ATOM	982	CB	GLN	A	136	48.317	35.145	47.306	1.00	12.71	A
ATOM	983	CG	GLN	A	136	47.892	36.594	47.337	1.00	19.42	A

FIGURE 5 (continued)

18 / 46

ATOM	984	CD	GLN	A	136	48.999	37.566	46.905	1.00	23.10	A
ATOM	985	OE1	GLN	A	136	49.620	37.403	45.858	1.00	23.52	A
ATOM	986	NE2	GLN	A	136	49.233	38.585	47.714	1.00	30.84	A
ATOM	987	C	GLN	A	136	46.105	34.023	47.053	1.00	9.51	A
ATOM	988	O	GLN	A	136	46.254	33.639	45.921	1.00	9.81	A
ATOM	989	N	VAL	A	137	44.911	34.303	47.552	1.00	8.18	A
ATOM	990	CA	VAL	A	137	43.717	34.161	46.733	1.00	4.96	A
ATOM	991	CB	VAL	A	137	42.470	33.907	47.657	1.00	8.36	A
ATOM	992	CG1	VAL	A	137	41.176	34.014	46.855	1.00	5.20	A
ATOM	993	CG2	VAL	A	137	42.589	32.543	48.294	1.00	10.61	A
ATOM	994	C	VAL	A	137	43.442	35.380	45.837	1.00	9.91	A
ATOM	995	O	VAL	A	137	43.555	36.534	46.284	1.00	9.14	A
ATOM	996	N	VAL	A	138	43.124	35.114	44.566	1.00	7.01	A
ATOM	997	CA	VAL	A	138	42.735	36.134	43.600	1.00	8.67	A
ATOM	998	CB	VAL	A	138	43.437	35.976	42.226	1.00	9.91	A
ATOM	999	CG1	VAL	A	138	42.983	37.092	41.301	1.00	11.71	A
ATOM	1000	CG2	VAL	A	138	44.947	36.068	42.394	1.00	18.67	A
ATOM	1001	C	VAL	A	138	41.237	35.914	43.386	1.00	7.40	A
ATOM	1002	O	VAL	A	138	40.791	34.775	43.196	1.00	7.75	A
ATOM	1003	N	TYR	A	139	40.452	36.987	43.435	1.00	9.87	A
ATOM	1004	CA	TYR	A	139	39.009	36.871	43.256	1.00	9.42	A
ATOM	1005	CB	TYR	A	139	38.303	36.902	44.625	1.00	8.26	A
ATOM	1006	CG	TYR	A	139	38.509	38.192	45.389	1.00	9.37	A
ATOM	1007	CD1	TYR	A	139	37.570	39.211	45.322	1.00	8.61	A
ATOM	1008	CE1	TYR	A	139	37.748	40.424	46.013	1.00	9.72	A
ATOM	1009	CD2	TYR	A	139	39.659	38.397	46.177	1.00	9.71	A
ATOM	1010	CE2	TYR	A	139	39.853	39.616	46.878	1.00	12.90	A
ATOM	1011	CZ	TYR	A	139	38.890	40.623	46.786	1.00	15.66	A
ATOM	1012	OH	TYR	A	139	39.045	41.829	47.459	1.00	8.23	A
ATOM	1013	C	TYR	A	139	38.507	38.006	42.381	1.00	8.45	A
ATOM	1014	O	TYR	A	139	39.246	38.947	42.099	1.00	8.15	A
ATOM	1015	N	ARG	A	140	37.259	37.899	41.935	1.00	8.93	A
ATOM	1016	CA	ARG	A	140	36.660	38.903	41.070	1.00	7.41	A
ATOM	1017	CB	ARG	A	140	35.514	38.296	40.243	1.00	10.32	A
ATOM	1018	CG	ARG	A	140	35.991	37.317	39.148	1.00	5.86	A
ATOM	1019	CD	ARG	A	140	36.556	38.103	37.948	1.00	5.80	A
ATOM	1020	NE	ARG	A	140	35.502	38.821	37.218	1.00	7.23	A
ATOM	1021	CZ	ARG	A	140	34.659	38.232	36.376	1.00	11.87	A
ATOM	1022	NH1	ARG	A	140	34.748	36.918	36.152	1.00	5.93	A
ATOM	1023	NH2	ARG	A	140	33.715	38.952	35.769	1.00	8.31	A
ATOM	1024	C	ARG	A	140	36.129	40.063	41.895	1.00	8.44	A
ATOM	1025	O	ARG	A	140	35.327	39.896	42.832	1.00	8.91	A
ATOM	1026	N	ALA	A	141	36.583	41.242	41.523	1.00	8.44	A
ATOM	1027	CA	ALA	A	141	36.198	42.471	42.206	1.00	8.99	A
ATOM	1028	CB	ALA	A	141	37.121	43.579	41.761	1.00	12.40	A
ATOM	1029	C	ALA	A	141	34.748	42.895	41.975	1.00	11.15	A
ATOM	1030	O	ALA	A	141	34.091	43.421	42.878	1.00	9.17	A
ATOM	1031	N	GLU	A	142	34.258	42.679	40.765	1.00	10.41	A
ATOM	1032	CA	GLU	A	142	32.912	43.110	40.401	1.00	11.28	A
ATOM	1033	CB	GLU	A	142	32.944	43.735	38.995	1.00	11.17	A
ATOM	1034	CG	GLU	A	142	32.968	42.720	37.800	1.00	16.02	A
ATOM	1035	CD	GLU	A	142	34.319	41.984	37.551	1.00	14.71	A
ATOM	1036	OE1	GLU	A	142	35.102	41.758	38.492	1.00	20.26	A
ATOM	1037	OE2	GLU	A	142	34.582	41.608	36.382	1.00	15.07	A
ATOM	1038	C	GLU	A	142	31.854	42.001	40.428	1.00	15.45	A
ATOM	1039	O	GLU	A	142	32.160	40.827	40.689	1.00	11.17	A
ATOM	1040	N	VAL	A	143	30.604	42.399	40.170	1.00	13.82	A
ATOM	1041	CA	VAL	A	143	29.474	41.461	40.114	1.00	12.65	A
ATOM	1042	CB	VAL	A	143	28.155	42.192	39.792	1.00	12.26	A
ATOM	1043	CG1	VAL	A	143	27.052	41.196	39.668	1.00	17.81	A
ATOM	1044	CG2	VAL	A	143	27.822	43.174	40.870	1.00	18.80	A
ATOM	1045	C	VAL	A	143	29.770	40.456	38.996	1.00	12.06	A
ATOM	1046	O	VAL	A	143	29.785	40.814	37.811	1.00	10.75	A
ATOM	1047	N	SER	A	144	29.972	39.198	39.388	1.00	10.21	A
ATOM	1048	CA	SER	A	144	30.352	38.119	38.462	1.00	6.60	A
ATOM	1049	CB	SER	A	144	31.822	37.764	38.758	1.00	8.21	A
ATOM	1050	OG	SER	A	144	32.188	36.468	38.328	1.00	8.64	A
ATOM	1051	C	SER	A	144	29.499	36.834	38.512	1.00	7.57	A
ATOM	1052	O	SER	A	144	29.166	36.346	39.601	1.00	8.05	A
ATOM	1053	N	GLY	A	145	29.168	36.303	37.330	1.00	5.34	A
ATOM	1054	CA	GLY	A	145	28.437	35.047	37.226	1.00	7.72	A
ATOM	1055	C	GLY	A	145	29.335	33.884	37.638	1.00	7.84	A
ATOM	1056	O	GLY	A	145	28.873	32.870	38.197	1.00	6.69	A
ATOM	1057	N	THR	A	146	30.628	34.001	37.357	1.00	6.57	A
ATOM	1058	CA	THR	A	146	31.574	32.953	37.758	1.00	6.39	A
ATOM	1059	CB	THR	A	146	33.012	33.263	37.279	1.00	9.37	A

FIGURE 5 (continued)

19 / 46

ATOM	1060	OG1	THR	A	146	33.026	33.463	35.855	1.00	8.49	A
ATOM	1061	CG2	THR	A	146	33.928	32.087	37.613	1.00	11.25	A
ATOM	1062	C	THR	A	146	31.569	32.892	39.294	1.00	8.02	A
ATOM	1063	O	THR	A	146	31.601	31.802	39.888	1.00	8.00	A
ATOM	1064	N	THR	A	147	31.551	34.064	39.930	1.00	6.33	A
ATOM	1065	CA	THR	A	147	31.483	34.131	41.394	1.00	8.35	A
ATOM	1066	CB	THR	A	147	31.554	35.591	41.921	1.00	6.29	A
ATOM	1067	OG1	THR	A	147	32.834	36.161	41.624	1.00	7.92	A
ATOM	1068	CG2	THR	A	147	31.373	35.602	43.450	1.00	8.46	A
ATOM	1069	C	THR	A	147	30.175	33.486	41.885	1.00	5.86	A
ATOM	1070	O	THR	A	147	30.172	32.745	42.883	1.00	7.90	A
ATOM	1071	N	GLU	A	148	29.059	33.751	41.198	1.00	5.81	A
ATOM	1072	CA	GLU	A	148	27.786	33.131	41.592	1.00	5.50	A
ATOM	1073	CB	GLU	A	148	26.644	33.653	40.710	1.00	6.06	A
ATOM	1074	CG	GLU	A	148	25.284	33.004	41.058	1.00	10.99	A
ATOM	1075	CD	GLU	A	148	24.076	33.737	40.457	1.00	12.04	A
ATOM	1076	OE1	GLU	A	148	23.920	34.966	40.685	1.00	9.92	A
ATOM	1077	OE2	GLU	A	148	23.271	33.078	39.765	1.00	13.03	A
ATOM	1078	C	GLU	A	148	27.846	31.591	41.491	1.00	6.20	A
ATOM	1079	O	GLU	A	148	27.419	30.866	42.408	1.00	7.44	A
ATOM	1080	N	LEU	A	149	28.318	31.077	40.359	1.00	4.66	A
ATOM	1081	CA	LEU	A	149	28.442	29.616	40.196	1.00	6.87	A
ATOM	1082	CB	LEU	A	149	29.011	29.301	38.807	1.00	7.74	A
ATOM	1083	CG	LEU	A	149	28.105	29.569	37.591	1.00	8.75	A
ATOM	1084	CD1	LEU	A	149	28.878	29.218	36.342	1.00	10.50	A
ATOM	1085	CD2	LEU	A	149	26.804	28.721	37.678	1.00	9.52	A
ATOM	1086	C	LEU	A	149	29.376	28.980	41.254	1.00	7.07	A
ATOM	1087	O	LEU	A	149	29.127	27.865	41.754	1.00	7.65	A
ATOM	1088	N	PHE	A	150	30.473	29.670	41.568	1.00	8.71	A
ATOM	1089	CA	PHE	A	150	31.459	29.183	42.540	1.00	7.06	A
ATOM	1090	CB	PHE	A	150	32.752	30.021	42.427	1.00	6.97	A
ATOM	1091	CG	PHE	A	150	33.884	29.551	43.325	1.00	9.24	A
ATOM	1092	CD1	PHE	A	150	34.313	28.225	43.305	1.00	10.27	A
ATOM	1093	CD2	PHE	A	150	34.557	30.455	44.138	1.00	12.03	A
ATOM	1094	CE1	PHE	A	150	35.411	27.803	44.081	1.00	12.21	A
ATOM	1095	CE2	PHE	A	150	35.657	30.050	44.920	1.00	11.31	A
ATOM	1096	CZ	PHE	A	150	36.083	28.721	44.890	1.00	10.56	A
ATOM	1097	C	PHE	A	150	30.936	29.217	43.987	1.00	7.58	A
ATOM	1098	O	PHE	A	150	31.060	28.236	44.709	1.00	6.52	A
ATOM	1099	N	THR	A	151	30.350	30.334	44.409	1.00	7.57	A
ATOM	1100	CA	THR	A	151	29.836	30.437	45.770	1.00	8.97	A
ATOM	1101	CB	THR	A	151	29.548	31.938	46.193	1.00	9.78	A
ATOM	1102	OG1	THR	A	151	28.580	32.526	45.314	1.00	8.77	A
ATOM	1103	CG2	THR	A	151	30.826	32.744	46.152	1.00	7.96	A
ATOM	1104	C	THR	A	151	28.588	29.588	45.988	1.00	7.22	A
ATOM	1105	O	THR	A	151	28.274	29.245	47.131	1.00	7.49	A
ATOM	1106	N	ARG	A	152	27.873	29.229	44.916	1.00	5.13	A
ATOM	1107	CA	ARG	A	152	26.715	28.351	45.099	1.00	9.17	A
ATOM	1108	CB	ARG	A	152	25.914	28.189	43.796	1.00	9.15	A
ATOM	1109	CG	ARG	A	152	24.606	27.376	43.974	1.00	10.79	A
ATOM	1110	CD	ARG	A	152	23.671	27.529	42.755	1.00	17.61	A
ATOM	1111	NE	ARG	A	152	23.071	28.868	42.641	1.00	14.93	A
ATOM	1112	CZ	ARG	A	152	23.188	29.662	41.577	1.00	16.78	A
ATOM	1113	NH1	ARG	A	152	22.605	30.860	41.565	1.00	11.71	A
ATOM	1114	NH2	ARG	A	152	23.885	29.265	40.518	1.00	11.02	A
ATOM	1115	C	ARG	A	152	27.274	27.007	45.557	1.00	7.79	A
ATOM	1116	O	ARG	A	152	26.671	26.313	46.389	1.00	5.08	A
ATOM	1117	N	PHE	A	153	28.436	26.639	45.017	1.00	6.70	A
ATOM	1118	CA	PHE	A	153	29.101	25.395	45.413	1.00	9.70	A
ATOM	1119	CB	PHE	A	153	30.280	25.059	44.478	1.00	7.27	A
ATOM	1120	CG	PHE	A	153	30.974	23.747	44.812	1.00	6.93	A
ATOM	1121	CD1	PHE	A	153	30.451	22.532	44.389	1.00	9.41	A
ATOM	1122	CD2	PHE	A	153	32.134	23.738	45.592	1.00	9.61	A
ATOM	1123	CE1	PHE	A	153	31.069	21.315	44.747	1.00	11.43	A
ATOM	1124	CE2	PHE	A	153	32.764	22.534	45.959	1.00	13.90	A
ATOM	1125	CZ	PHE	A	153	32.229	21.323	45.537	1.00	11.19	A
ATOM	1126	C	PHE	A	153	29.640	25.503	46.842	1.00	8.50	A
ATOM	1127	O	PHE	A	153	29.455	24.586	47.638	1.00	8.41	A
ATOM	1128	N	LEU	A	154	30.320	26.599	47.167	1.00	6.84	A
ATOM	1129	CA	LEU	A	154	30.877	26.752	48.521	1.00	6.20	A
ATOM	1130	CB	LEU	A	154	31.672	28.060	48.657	1.00	6.23	A
ATOM	1131	CG	LEU	A	154	32.876	28.250	47.720	1.00	6.30	A
ATOM	1132	CD1	LEU	A	154	33.543	29.583	48.020	1.00	9.48	A
ATOM	1133	CD2	LEU	A	154	33.893	27.117	47.886	1.00	6.15	A
ATOM	1134	C	LEU	A	154	29.762	26.737	49.564	1.00	6.13	A
ATOM	1135	O	LEU	A	154	29.912	26.170	50.641	1.00	9.16	A

FIGURE 5 (continued)

20 / 46

ATOM	1136	N	ASN	A	155	28.652	27.376	49.233	1.00	5.19	A
ATOM	1137	CA	ASN	A	155	27.493	27.430	50.116	1.00	6.32	A
ATOM	1138	CB	ASN	A	155	26.406	28.314	49.486	1.00	11.33	A
ATOM	1139	CG	ASN	A	155	25.093	28.294	50.274	1.00	14.59	A
ATOM	1140	OD1	ASN	A	155	24.149	27.596	49.906	1.00	9.21	A
ATOM	1141	ND2	ASN	A	155	25.034	29.062	51.361	1.00	8.23	A
ATOM	1142	C	ASN	A	155	26.929	26.042	50.363	1.00	8.76	A
ATOM	1143	O	ASN	A	155	26.465	25.712	51.465	1.00	8.00	A
ATOM	1144	N	ALA	A	156	26.965	25.203	49.336	1.00	8.80	A
ATOM	1145	CA	ALA	A	156	26.418	23.867	49.493	1.00	7.63	A
ATOM	1146	CB	ALA	A	156	26.068	23.300	48.119	1.00	8.06	A
ATOM	1147	C	ALA	A	156	27.336	22.882	50.222	1.00	12.23	A
ATOM	1148	O	ALA	A	156	26.854	22.037	50.994	1.00	9.62	A
ATOM	1149	N	LYS	A	157	28.646	23.029	50.015	1.00	9.93	A
ATOM	1150	CA	LYS	A	157	29.623	22.064	50.537	1.00	10.69	A
ATOM	1151	CB	LYS	A	157	30.437	21.527	49.352	1.00	14.97	A
ATOM	1152	CG	LYS	A	157	29.604	20.877	48.227	1.00	13.56	A
ATOM	1153	CD	LYS	A	157	28.855	19.640	48.729	1.00	16.77	A
ATOM	1154	CE	LYS	A	157	28.357	18.784	47.575	1.00	22.67	A
ATOM	1155	NZ	LYS	A	157	27.652	17.546	48.069	1.00	21.73	A
ATOM	1156	C	LYS	A	157	30.611	22.438	51.638	1.00	8.73	A
ATOM	1157	O	LYS	A	157	31.215	21.552	52.245	1.00	11.63	A
ATOM	1158	N	CYS	A	158	30.821	23.725	51.876	1.00	8.12	A
ATOM	1159	CA	CYS	A	158	31.759	24.132	52.916	1.00	8.20	A
ATOM	1160	C	CYS	A	158	30.974	24.252	54.207	1.00	9.14	A
ATOM	1161	O	CYS	A	158	30.648	25.349	54.661	1.00	10.53	A
ATOM	1162	CB	CYS	A	158	32.390	25.464	52.537	1.00	10.13	A
ATOM	1163	SG	CYS	A	158	33.331	25.358	50.982	1.00	11.82	A
ATOM	1164	N	THR	A	159	30.699	23.108	54.822	1.00	8.92	A
ATOM	1165	CA	THR	A	159	29.856	23.091	56.017	1.00	6.75	A
ATOM	1166	CB	THR	A	159	28.850	21.933	55.903	1.00	10.13	A
ATOM	1167	OG1	THR	A	159	29.551	20.690	55.987	1.00	12.88	A
ATOM	1168	CG2	THR	A	159	28.146	21.989	54.527	1.00	14.84	A
ATOM	1169	C	THR	A	159	30.545	23.021	57.361	1.00	8.62	A
ATOM	1170	O	THR	A	159	29.878	22.956	58.398	1.00	7.39	A
ATOM	1171	N	THR	A	160	31.875	23.038	57.358	1.00	8.39	A
ATOM	1172	CA	THR	A	160	32.603	22.980	58.612	1.00	9.53	A
ATOM	1173	CB	THR	A	160	33.194	21.558	58.889	1.00	8.99	A
ATOM	1174	OG1	THR	A	160	34.011	21.140	57.788	1.00	12.55	A
ATOM	1175	CG2	THR	A	160	32.083	20.559	59.114	1.00	11.60	A
ATOM	1176	C	THR	A	160	33.727	24.010	58.712	1.00	10.20	A
ATOM	1177	O	THR	A	160	34.774	23.739	59.314	1.00	8.76	A
ATOM	1178	N	GLN	A	161	33.523	25.189	58.121	1.00	8.66	A
ATOM	1179	CA	GLN	A	161	34.525	26.260	58.254	1.00	9.46	A
ATOM	1180	CB	GLN	A	161	34.564	27.121	56.989	1.00	9.58	A
ATOM	1181	CG	GLN	A	161	34.956	26.309	55.742	1.00	7.83	A
ATOM	1182	CD	GLN	A	161	36.305	25.608	55.936	1.00	10.81	A
ATOM	1183	OE1	GLN	A	161	36.429	24.396	55.758	1.00	12.80	A
ATOM	1184	NE2	GLN	A	161	37.306	26.374	56.313	1.00	10.64	A
ATOM	1185	C	GLN	A	161	34.058	27.096	59.449	1.00	8.71	A
ATOM	1186	O	GLN	A	161	32.979	26.866	59.960	1.00	8.58	A
ATOM	1187	N	PRO	A	162	34.870	28.047	59.928	1.00	11.51	A
ATOM	1188	CD	PRO	A	162	36.316	28.193	59.693	1.00	10.65	A
ATOM	1189	CA	PRO	A	162	34.433	28.869	61.071	1.00	9.23	A
ATOM	1190	CB	PRO	A	162	35.631	29.780	61.326	1.00	11.89	A
ATOM	1191	CG	PRO	A	162	36.786	28.884	60.979	1.00	14.39	A
ATOM	1192	C	PRO	A	162	33.171	29.660	60.727	1.00	10.67	A
ATOM	1193	O	PRO	A	162	32.280	29.838	61.567	1.00	12.32	A
ATOM	1194	N	GLY	A	163	33.112	30.158	59.492	1.00	8.94	A
ATOM	1195	CA	GLY	A	163	31.943	30.903	59.040	1.00	11.83	A
ATOM	1196	C	GLY	A	163	31.307	30.149	57.883	1.00	11.53	A
ATOM	1197	O	GLY	A	163	31.687	28.989	57.628	1.00	9.27	A
ATOM	1198	N	THR	A	164	30.359	30.781	57.178	1.00	7.79	A
ATOM	1199	CA	THR	A	164	29.698	30.140	56.039	1.00	10.06	A
ATOM	1200	CB	THR	A	164	28.213	29.775	56.347	1.00	9.77	A
ATOM	1201	OG1	THR	A	164	27.565	30.914	56.934	1.00	12.97	A
ATOM	1202	CG2	THR	A	164	28.119	28.585	57.328	1.00	7.94	A
ATOM	1203	C	THR	A	164	29.696	31.081	54.837	1.00	10.41	A
ATOM	1204	O	THR	A	164	29.786	32.301	55.001	1.00	7.96	A
ATOM	1205	N	PHE	A	165	29.571	30.507	53.637	1.00	7.32	A
ATOM	1206	CA	PHE	A	165	29.551	31.275	52.395	1.00	9.34	A
ATOM	1207	CB	PHE	A	165	30.321	30.541	51.299	1.00	8.51	A
ATOM	1208	CG	PHE	A	165	31.799	30.451	51.539	1.00	7.69	A
ATOM	1209	CD1	PHE	A	165	32.659	31.455	51.096	1.00	8.05	A
ATOM	1210	CD2	PHE	A	165	32.338	29.338	52.181	1.00	10.52	A
ATOM	1211	CE1	PHE	A	165	34.062	31.349	51.288	1.00	6.48	A

FIGURE 5 (continued)

21 / 46

ATOM	1212	CE2	PHE	A	165	33.720	29.214	52.385	1.00	6.44	A
ATOM	1213	CZ	PHE	A	165	34.591	30.221	51.935	1.00	7.86	A
ATOM	1214	C	PHE	A	165	28.135	31.467	51.854	1.00	10.39	A
ATOM	1215	O	PHE	A	165	27.428	30.485	51.648	1.00	11.83	A
ATOM	1216	N	ALA	A	166	27.738	32.712	51.601	1.00	8.80	A
ATOM	1217	CA	ALA	A	166	26.424	33.000	51.006	1.00	10.97	A
ATOM	1218	CB	ALA	A	166	25.942	34.397	51.423	1.00	10.57	A
ATOM	1219	C	ALA	A	166	26.593	32.960	49.483	1.00	10.58	A
ATOM	1220	O	ALA	A	166	27.694	33.182	48.968	1.00	7.60	A
ATOM	1221	N	VAL	A	167	25.516	32.668	48.766	1.00	9.26	A
ATOM	1222	CA	VAL	A	167	25.572	32.658	47.303	1.00	7.71	A
ATOM	1223	CB	VAL	A	167	24.384	31.924	46.686	1.00	7.77	A
ATOM	1224	CG1	VAL	A	167	24.546	31.870	45.159	1.00	8.04	A
ATOM	1225	CG2	VAL	A	167	24.283	30.511	47.265	1.00	10.61	A
ATOM	1226	C	VAL	A	167	25.473	34.123	46.875	1.00	8.91	A
ATOM	1227	O	VAL	A	167	24.523	34.816	47.244	1.00	7.79	A
ATOM	1228	N	THR	A	168	26.408	34.580	46.048	1.00	8.13	A
ATOM	1229	CA	THR	A	168	26.411	35.974	45.653	1.00	6.66	A
ATOM	1230	CB	THR	A	168	27.060	36.810	46.769	1.00	13.46	A
ATOM	1231	OG1	THR	A	168	27.129	38.188	46.370	1.00	12.35	A
ATOM	1232	CG2	THR	A	168	28.478	36.311	47.040	1.00	12.28	A
ATOM	1233	C	THR	A	168	27.228	36.178	44.375	1.00	11.69	A
ATOM	1234	O	THR	A	168	27.960	35.282	43.947	1.00	11.22	A
ATOM	1235	N	THR	A	169	27.106	37.352	43.770	1.00	9.36	A
ATOM	1236	CA	THR	A	169	27.888	37.641	42.580	1.00	5.90	A
ATOM	1237	CB	THR	A	169	27.074	38.484	41.565	1.00	11.79	A
ATOM	1238	OG1	THR	A	169	26.724	39.739	42.169	1.00	9.77	A
ATOM	1239	CG2	THR	A	169	25.811	37.747	41.128	1.00	12.13	A
ATOM	1240	C	THR	A	169	29.156	38.450	42.953	1.00	9.03	A
ATOM	1241	O	THR	A	169	30.000	38.712	42.099	1.00	8.64	A
ATOM	1242	N	VAL	A	170	29.279	38.848	44.224	1.00	11.21	A
ATOM	1243	CA	VAL	A	170	30.430	39.641	44.680	1.00	11.07	A
ATOM	1244	CB	VAL	A	170	29.944	41.003	45.248	1.00	8.64	A
ATOM	1245	CG1	VAL	A	170	29.433	41.863	44.106	1.00	8.12	A
ATOM	1246	CG2	VAL	A	170	28.802	40.805	46.208	1.00	14.20	A
ATOM	1247	C	VAL	A	170	31.158	38.830	45.741	1.00	10.94	A
ATOM	1248	O	VAL	A	170	30.694	38.747	46.859	1.00	11.12	A
ATOM	1249	N	PHE	A	171	32.305	38.247	45.386	1.00	11.66	A
ATOM	1250	CA	PHE	A	171	33.003	37.367	46.312	1.00	9.52	A
ATOM	1251	CB	PHE	A	171	34.279	36.775	45.677	1.00	8.67	A
ATOM	1252	CG	PHE	A	171	34.940	35.686	46.519	1.00	10.69	A
ATOM	1253	CD1	PHE	A	171	36.009	35.978	47.358	1.00	9.84	A
ATOM	1254	CD2	PHE	A	171	34.457	34.377	46.502	1.00	14.44	A
ATOM	1255	CE1	PHE	A	171	36.593	34.986	48.184	1.00	8.85	A
ATOM	1256	CE2	PHE	A	171	35.024	33.377	47.311	1.00	12.76	A
ATOM	1257	CZ	PHE	A	171	36.096	33.686	48.158	1.00	12.60	A
ATOM	1258	C	PHE	A	171	33.353	37.977	47.661	1.00	12.55	A
ATOM	1259	O	PHE	A	171	33.292	37.294	48.679	1.00	7.64	A
ATOM	1260	N	ALA	A	172	33.704	39.257	47.677	1.00	6.57	A
ATOM	1261	CA	ALA	A	172	34.088	39.865	48.946	1.00	9.02	A
ATOM	1262	CB	ALA	A	172	34.655	41.279	48.721	1.00	9.26	A
ATOM	1263	C	ALA	A	172	32.948	39.885	49.957	1.00	11.22	A
ATOM	1264	O	ALA	A	172	33.188	40.071	51.155	1.00	10.96	A
ATOM	1265	N	ASN	A	173	31.714	39.677	49.493	1.00	8.23	A
ATOM	1266	CA	ASN	A	173	30.563	39.651	50.409	1.00	10.55	A
ATOM	1267	CB	ASN	A	173	29.361	40.396	49.822	1.00	11.87	A
ATOM	1268	CG	ASN	A	173	29.628	41.862	49.606	1.00	13.88	A
ATOM	1269	OD1	ASN	A	173	30.289	42.512	50.412	1.00	13.36	A
ATOM	1270	ND2	ASN	A	173	29.098	42.398	48.515	1.00	16.29	A
ATOM	1271	C	ASN	A	173	30.062	38.245	50.759	1.00	13.21	A
ATOM	1272	O	ASN	A	173	29.077	38.109	51.498	1.00	10.89	A
ATOM	1273	N	SER	A	174	30.716	37.212	50.238	1.00	7.67	A
ATOM	1274	CA	SER	A	174	30.250	35.859	50.468	1.00	9.24	A
ATOM	1275	CB	SER	A	174	30.869	34.905	49.429	1.00	9.01	A
ATOM	1276	OG	SER	A	174	30.359	33.580	49.598	1.00	8.15	A
ATOM	1277	C	SER	A	174	30.440	35.250	51.863	1.00	7.73	A
ATOM	1278	O	SER	A	174	29.480	34.822	52.506	1.00	8.54	A
ATOM	1279	N	TYR	A	175	31.684	35.160	52.303	1.00	6.67	A
ATOM	1280	CA	TYR	A	175	31.978	34.535	53.599	1.00	6.35	A
ATOM	1281	CB	TYR	A	175	33.493	34.371	53.735	1.00	7.83	A
ATOM	1282	CG	TYR	A	175	33.928	33.429	54.847	1.00	6.19	A
ATOM	1283	CD1	TYR	A	175	34.845	33.842	55.825	1.00	9.13	A
ATOM	1284	CE1	TYR	A	175	35.315	32.938	56.811	1.00	7.78	A
ATOM	1285	CD2	TYR	A	175	33.481	32.102	54.879	1.00	6.63	A
ATOM	1286	CE2	TYR	A	175	33.939	31.206	55.856	1.00	9.07	A
ATOM	1287	CZ	TYR	A	175	34.859	31.633	56.812	1.00	11.83	A

FIGURE 5 (continued)

22 / 46

ATOM	1288	OH	TYR	A	175	35.348	30.731	57.746	1.00	8.85	A
ATOM	1289	C	TYR	A	175	31.424	35.365	54.761	1.00	12.71	A
ATOM	1290	O	TYR	A	175	31.649	36.556	54.806	1.00	7.92	A
ATOM	1291	N	SER	A	176	30.695	34.727	55.683	1.00	9.13	A
ATOM	1292	CA	SER	A	176	30.104	35.431	56.828	1.00	9.94	A
ATOM	1293	CB	SER	A	176	29.372	34.433	57.737	1.00	11.72	A
ATOM	1294	OG	SER	A	176	30.248	33.426	58.245	1.00	9.80	A
ATOM	1295	C	SER	A	176	31.092	36.247	57.659	1.00	11.68	A
ATOM	1296	O	SER	A	176	30.737	37.302	58.184	1.00	12.94	A
ATOM	1297	N	LEU	A	177	32.332	35.787	57.788	1.00	10.90	A
ATOM	1298	CA	LEU	A	177	33.303	36.559	58.561	1.00	12.59	A
ATOM	1299	CB	LEU	A	177	34.231	35.613	59.349	1.00	14.55	A
ATOM	1300	CG	LEU	A	177	33.537	34.649	60.324	1.00	15.21	A
ATOM	1301	CD1	LEU	A	177	34.579	33.649	60.872	1.00	18.41	A
ATOM	1302	CD2	LEU	A	177	32.856	35.452	61.476	1.00	11.73	A
ATOM	1303	C	LEU	A	177	34.139	37.522	57.692	1.00	13.68	A
ATOM	1304	O	LEU	A	177	35.126	38.104	58.163	1.00	12.71	A
ATOM	1305	N	GLY	A	178	33.754	37.680	56.434	1.00	9.18	A
ATOM	1306	CA	GLY	A	178	34.475	38.585	55.541	1.00	12.34	A
ATOM	1307	C	GLY	A	178	35.803	38.098	54.975	1.00	12.74	A
ATOM	1308	O	GLY	A	178	36.205	36.939	55.208	1.00	13.97	A
ATOM	1309	N	LEU	A	179	36.492	38.974	54.224	1.00	9.84	A
ATOM	1310	CA	LEU	A	179	37.787	38.610	53.621	1.00	10.63	A
ATOM	1311	CB	LEU	A	179	38.078	39.437	52.350	1.00	11.33	A
ATOM	1312	CG	LEU	A	179	37.189	39.202	51.120	1.00	10.67	A
ATOM	1313	CD1	LEU	A	179	37.729	40.017	49.934	1.00	12.85	A
ATOM	1314	CD2	LEU	A	179	37.134	37.692	50.787	1.00	15.70	A
ATOM	1315	C	LEU	A	179	38.986	38.779	54.555	1.00	12.52	A
ATOM	1316	O	LEU	A	179	40.096	38.319	54.233	1.00	13.43	A
ATOM	1317	N	SER	A	180	38.788	39.426	55.702	1.00	13.88	A
ATOM	1318	CA	SER	A	180	39.910	39.635	56.612	1.00	17.84	A
ATOM	1319	CB	SER	A	180	39.438	40.187	57.954	1.00	23.37	A
ATOM	1320	OG	SER	A	180	39.006	41.521	57.770	1.00	30.75	A
ATOM	1321	C	SER	A	180	40.776	38.411	56.839	1.00	18.97	A
ATOM	1322	O	SER	A	180	41.990	38.527	56.856	1.00	16.57	A
ATOM	1323	N	PRO	A	181	40.170	37.223	57.010	1.00	17.96	A
ATOM	1324	CD	PRO	A	181	38.739	36.923	57.219	1.00	18.24	A
ATOM	1325	CA	PRO	A	181	40.989	36.023	57.228	1.00	19.35	A
ATOM	1326	CB	PRO	A	181	39.948	34.925	57.436	1.00	20.22	A
ATOM	1327	CG	PRO	A	181	38.804	35.657	58.063	1.00	20.57	A
ATOM	1328	C	PRO	A	181	41.927	35.697	56.063	1.00	24.47	A
ATOM	1329	O	PRO	A	181	42.893	34.943	56.237	1.00	26.18	A
ATOM	1330	N	LEU	A	182	41.646	36.251	54.880	1.00	17.84	A
ATOM	1331	CA	LEU	A	182	42.470	36.002	53.688	1.00	21.43	A
ATOM	1332	CB	LEU	A	182	41.615	36.019	52.410	1.00	20.15	A
ATOM	1333	CG	LEU	A	182	40.748	34.780	52.178	1.00	20.14	A
ATOM	1334	CD1	LEU	A	182	39.849	34.968	50.952	1.00	17.30	A
ATOM	1335	CD2	LEU	A	182	41.679	33.580	52.004	1.00	15.09	A
ATOM	1336	C	LEU	A	182	43.614	36.985	53.490	1.00	27.88	A
ATOM	1337	O	LEU	A	182	43.499	37.909	52.682	1.00	31.51	A
ATOM	1338	N	ALA	A	183	44.726	36.761	54.185	1.00	23.49	A
ATOM	1339	CA	ALA	A	183	45.893	37.639	54.073	1.00	26.24	A
ATOM	1340	CB	ALA	A	183	47.066	37.047	54.860	1.00	22.25	A
ATOM	1341	C	ALA	A	183	46.325	37.920	52.629	1.00	20.58	A
ATOM	1342	O	ALA	A	183	46.623	37.001	51.856	1.00	17.37	A
ATOM	1343	N	GLY	A	184	46.354	39.202	52.278	1.00	17.97	A
ATOM	1344	CA	GLY	A	184	46.762	39.603	50.949	1.00	17.46	A
ATOM	1345	C	GLY	A	184	45.908	39.186	49.755	1.00	12.78	A
ATOM	1346	O	GLY	A	184	46.413	39.159	48.636	1.00	15.39	A
ATOM	1347	N	ALA	A	185	44.634	38.878	49.956	1.00	12.15	A
ATOM	1348	CA	ALA	A	185	43.798	38.500	48.811	1.00	14.55	A
ATOM	1349	CB	ALA	A	185	42.374	38.212	49.271	1.00	14.22	A
ATOM	1350	C	ALA	A	185	43.812	39.649	47.795	1.00	16.74	A
ATOM	1351	O	ALA	A	185	43.780	40.826	48.181	1.00	15.66	A
ATOM	1352	N	VAL	A	186	43.836	39.300	46.507	1.00	9.90	A
ATOM	1353	CA	VAL	A	186	43.880	40.276	45.419	1.00	11.92	A
ATOM	1354	CB	VAL	A	186	45.093	39.969	44.484	1.00	14.98	A
ATOM	1355	CG1	VAL	A	186	45.026	40.816	43.229	1.00	13.29	A
ATOM	1356	CG2	VAL	A	186	46.398	40.226	45.244	1.00	19.64	A
ATOM	1357	C	VAL	A	186	42.608	40.254	44.571	1.00	11.79	A
ATOM	1358	O	VAL	A	186	42.152	39.182	44.149	1.00	11.34	A
ATOM	1359	N	ALA	A	187	42.035	41.430	44.331	1.00	11.06	A
ATOM	1360	CA	ALA	A	187	40.829	41.543	43.508	1.00	10.57	A
ATOM	1361	CB	ALA	A	187	39.897	42.606	44.096	1.00	12.53	A
ATOM	1362	C	ALA	A	187	41.211	41.923	42.079	1.00	13.16	A
ATOM	1363	O	ALA	A	187	42.128	42.736	41.876	1.00	14.58	A

FIGURE 5 (continued)

23 / 46

ATOM	1364	N	ALA	A	188	40.543	41.328	41.085	1.00	8.38	A
ATOM	1365	CA	ALA	A	188	40.832	41.672	39.672	1.00	8.09	A
ATOM	1366	CB	ALA	A	188	41.725	40.609	39.018	1.00	10.94	A
ATOM	1367	C	ALA	A	188	39.515	41.759	38.913	1.00	9.75	A
ATOM	1368	O	ALA	A	188	38.510	41.196	39.349	1.00	10.74	A
ATOM	1369	N	ILE	A	189	39.543	42.434	37.766	1.00	10.19	A
ATOM	1370	CA	ILE	A	189	38.355	42.646	36.936	1.00	9.71	A
ATOM	1371	CB	ILE	A	189	38.300	44.126	36.487	1.00	14.84	A
ATOM	1372	CG2	ILE	A	189	37.056	44.394	35.606	1.00	12.56	A
ATOM	1373	CG1	ILE	A	189	38.247	45.007	37.720	1.00	13.85	A
ATOM	1374	CD1	ILE	A	189	36.964	44.848	38.520	1.00	20.17	A
ATOM	1375	C	ILE	A	189	38.307	41.760	35.705	1.00	11.18	A
ATOM	1376	O	ILE	A	189	39.260	41.715	34.930	1.00	12.80	A
ATOM	1377	N	GLY	A	190	37.185	41.062	35.518	1.00	12.93	A
ATOM	1378	CA	GLY	A	190	37.039	40.181	34.368	1.00	9.66	A
ATOM	1379	C	GLY	A	190	37.836	38.881	34.432	1.00	11.20	A
ATOM	1380	O	GLY	A	190	38.763	38.745	35.238	1.00	12.00	A
ATOM	1381	N	SER	A	191	37.494	37.919	33.570	1.00	12.31	A
ATOM	1382	CA	SER	A	191	38.216	36.644	33.539	1.00	11.69	A
ATOM	1383	CB	SER	A	191	37.530	35.671	32.568	1.00	8.59	A
ATOM	1384	OG	SER	A	191	36.224	35.299	33.026	1.00	10.08	A
ATOM	1385	C	SER	A	191	39.678	36.896	33.104	1.00	14.30	A
ATOM	1386	O	SER	A	191	40.612	36.295	33.638	1.00	11.39	A
ATOM	1387	N	VAL	A	192	39.880	37.809	32.156	1.00	11.76	A
ATOM	1388	CA	VAL	A	192	41.235	38.101	31.704	1.00	14.84	A
ATOM	1389	CB	VAL	A	192	41.273	39.029	30.449	1.00	13.34	A
ATOM	1390	CG1	VAL	A	192	40.838	38.252	29.213	1.00	24.13	A
ATOM	1391	CG2	VAL	A	192	40.396	40.246	30.678	1.00	29.05	A
ATOM	1392	C	VAL	A	192	42.056	38.767	32.804	1.00	11.65	A
ATOM	1393	O	VAL	A	192	43.247	38.485	32.940	1.00	14.10	A
ATOM	1394	N	GLY	A	193	41.431	39.670	33.559	1.00	12.08	A
ATOM	1395	CA	GLY	A	193	42.149	40.344	34.626	1.00	12.16	A
ATOM	1396	C	GLY	A	193	42.575	39.354	35.700	1.00	14.30	A
ATOM	1397	O	GLY	A	193	43.652	39.486	36.291	1.00	9.20	A
ATOM	1398	N	VAL	A	194	41.725	38.369	35.976	1.00	9.32	A
ATOM	1399	CA	VAL	A	194	42.069	37.370	36.992	1.00	9.16	A
ATOM	1400	CB	VAL	A	194	40.845	36.459	37.341	1.00	7.74	A
ATOM	1401	CG1	VAL	A	194	41.309	35.168	38.071	1.00	8.55	A
ATOM	1402	CG2	VAL	A	194	39.873	37.247	38.259	1.00	11.33	A
ATOM	1403	C	VAL	A	194	43.256	36.524	36.530	1.00	10.65	A
ATOM	1404	O	VAL	A	194	44.158	36.255	37.318	1.00	10.00	A
ATOM	1405	N	MET	A	195	43.261	36.090	35.265	1.00	9.82	A
ATOM	1406	CA	MET	A	195	44.391	35.306	34.775	1.00	11.27	A
ATOM	1407	CB	MET	A	195	44.125	34.727	33.381	1.00	13.33	A
ATOM	1408	CG	MET	A	195	43.342	33.449	33.381	1.00	16.98	A
ATOM	1409	SD	MET	A	195	43.794	32.237	34.698	1.00	19.79	A
ATOM	1410	CE	MET	A	195	45.205	31.419	34.043	1.00	16.46	A
ATOM	1411	C	MET	A	195	45.672	36.118	34.719	1.00	12.67	A
ATOM	1412	O	MET	A	195	46.757	35.579	34.948	1.00	15.56	A
ATOM	1413	N	ALA	A	196	45.566	37.401	34.385	1.00	11.82	A
ATOM	1414	CA	ALA	A	196	46.750	38.239	34.346	1.00	15.74	A
ATOM	1415	CB	ALA	A	196	46.404	39.633	33.833	1.00	14.20	A
ATOM	1416	C	ALA	A	196	47.331	38.323	35.768	1.00	16.81	A
ATOM	1417	O	ALA	A	196	48.544	38.245	35.945	1.00	15.03	A
ATOM	1418	N	ALA	A	197	46.464	38.468	36.778	1.00	13.86	A
ATOM	1419	CA	ALA	A	197	46.939	38.538	38.151	1.00	13.25	A
ATOM	1420	CB	ALA	A	197	45.790	38.865	39.108	1.00	13.70	A
ATOM	1421	C	ALA	A	197	47.547	37.203	38.542	1.00	13.49	A
ATOM	1422	O	ALA	A	197	48.618	37.159	39.147	1.00	13.32	A
ATOM	1423	N	ASP	A	198	46.853	36.119	38.202	1.00	12.41	A
ATOM	1424	CA	ASP	A	198	47.326	34.777	38.547	1.00	16.61	A
ATOM	1425	CB	ASP	A	198	46.311	33.719	38.074	1.00	18.96	A
ATOM	1426	CG	ASP	A	198	46.605	32.327	38.629	1.00	29.19	A
ATOM	1427	OD1	ASP	A	198	46.440	32.107	39.857	1.00	32.24	A
ATOM	1428	OD2	ASP	A	198	47.004	31.449	37.834	1.00	34.04	A
ATOM	1429	C	ASP	A	198	48.699	34.509	37.928	1.00	17.95	A
ATOM	1430	O	ASP	A	198	49.570	33.942	38.585	1.00	18.27	A
ATOM	1431	N	ASN	A	199	48.900	34.941	36.684	1.00	16.24	A
ATOM	1432	CA	ASN	A	199	50.173	34.733	35.980	1.00	17.75	A
ATOM	1433	CB	ASN	A	199	49.941	34.565	34.478	1.00	19.50	A
ATOM	1434	CG	ASN	A	199	49.270	33.263	34.122	1.00	21.16	A
ATOM	1435	OD1	ASN	A	199	49.454	32.254	34.786	1.00	29.31	A
ATOM	1436	ND2	ASN	A	199	48.504	33.275	33.041	1.00	24.39	A
ATOM	1437	C	ASN	A	199	51.227	35.832	36.144	1.00	20.64	A
ATOM	1438	O	ASN	A	199	52.272	35.762	35.507	1.00	27.47	A
ATOM	1439	N	ASP	A	200	50.973	36.838	36.970	1.00	19.22	A

FIGURE 5 (continued)

24 / 46

ATOM	1440	CA	ASP	A	200	51.925	37.937	37.148	1.00	20.54	A
ATOM	1441	CB	ASP	A	200	51.350	38.985	38.092	1.00	22.32	A
ATOM	1442	CG	ASP	A	200	52.166	40.271	38.105	1.00	23.11	A
ATOM	1443	OD1	ASP	A	200	53.356	40.256	37.713	1.00	21.11	A
ATOM	1444	OD2	ASP	A	200	51.612	41.296	38.526	1.00	26.57	A
ATOM	1445	C	ASP	A	200	53.252	37.431	37.716	1.00	21.98	A
ATOM	1446	O	ASP	A	200	53.315	36.967	38.855	1.00	19.25	A
ATOM	1447	N	VAL	A	201	54.315	37.511	36.922	1.00	21.71	A
ATOM	1448	CA	VAL	A	201	55.611	37.033	37.390	1.00	24.01	A
ATOM	1449	CB	VAL	A	201	56.519	36.597	36.216	1.00	23.59	A
ATOM	1450	CG1	VAL	A	201	55.910	35.377	35.519	1.00	25.93	A
ATOM	1451	CG2	VAL	A	201	56.710	37.754	35.246	1.00	26.53	A
ATOM	1452	C	VAL	A	201	56.370	38.046	38.222	1.00	24.27	A
ATOM	1453	O	VAL	A	201	57.451	37.744	38.715	1.00	30.90	A
ATOM	1454	N	THR	A	202	55.817	39.241	38.402	1.00	23.14	A
ATOM	1455	CA	THR	A	202	56.511	40.251	39.190	1.00	23.53	A
ATOM	1456	CB	THR	A	202	56.216	41.664	38.696	1.00	22.33	A
ATOM	1457	OG1	THR	A	202	54.846	41.999	38.979	1.00	24.30	A
ATOM	1458	CG2	THR	A	202	56.489	41.759	37.210	1.00	25.94	A
ATOM	1459	C	THR	A	202	56.171	40.184	40.677	1.00	24.49	A
ATOM	1460	O	THR	A	202	56.543	41.073	41.444	1.00	25.68	A
ATOM	1461	N	THR	A	203	55.440	39.147	41.076	1.00	19.97	A
ATOM	1462	CA	THR	A	203	55.116	38.957	42.484	1.00	20.69	A
ATOM	1463	CB	THR	A	203	53.608	39.167	42.768	1.00	26.13	A
ATOM	1464	OG1	THR	A	203	52.825	38.196	42.047	1.00	25.13	A
ATOM	1465	CG2	THR	A	203	53.202	40.581	42.363	1.00	26.59	A
ATOM	1466	C	THR	A	203	55.523	37.521	42.834	1.00	17.47	A
ATOM	1467	O	THR	A	203	55.771	36.703	41.947	1.00	18.21	A
ATOM	1468	N	ALA	A	204	55.624	37.217	44.116	1.00	16.96	A
ATOM	1469	CA	ALA	A	204	56.011	35.867	44.528	1.00	16.26	A
ATOM	1470	CB	ALA	A	204	56.175	35.825	46.065	1.00	18.50	A
ATOM	1471	C	ALA	A	204	54.978	34.832	44.092	1.00	14.92	A
ATOM	1472	O	ALA	A	204	53.806	35.157	43.906	1.00	16.09	A
ATOM	1473	N	GLN	A	205	55.409	33.582	43.921	1.00	16.21	A
ATOM	1474	CA	GLN	A	205	54.483	32.501	43.560	1.00	16.27	A
ATOM	1475	CB	GLN	A	205	55.232	31.191	43.316	1.00	15.65	A
ATOM	1476	CG	GLN	A	205	56.103	31.148	42.097	1.00	22.41	A
ATOM	1477	CD	GLN	A	205	56.469	29.716	41.717	1.00	29.28	A
ATOM	1478	OE1	GLN	A	205	56.446	28.801	42.565	1.00	20.67	A
ATOM	1479	NE2	GLN	A	205	56.813	29.510	40.442	1.00	25.77	A
ATOM	1480	C	GLN	A	205	53.529	32.262	44.728	1.00	14.53	A
ATOM	1481	O	GLN	A	205	53.783	32.717	45.846	1.00	14.81	A
ATOM	1482	N	GLY	A	206	52.438	31.540	44.478	1.00	11.64	A
ATOM	1483	CA	GLY	A	206	51.509	31.236	45.554	1.00	11.46	A
ATOM	1484	C	GLY	A	206	50.042	31.518	45.284	1.00	11.44	A
ATOM	1485	O	GLY	A	206	49.162	31.067	46.046	1.00	9.87	A
ATOM	1486	N	ARG	A	207	49.764	32.236	44.199	1.00	7.71	A
ATOM	1487	CA	ARG	A	207	48.383	32.606	43.878	1.00	7.50	A
ATOM	1488	CB	ARG	A	207	48.364	33.763	42.863	1.00	9.66	A
ATOM	1489	CG	ARG	A	207	48.719	35.114	43.493	1.00	7.35	A
ATOM	1490	CD	ARG	A	207	48.774	36.286	42.497	1.00	6.76	A
ATOM	1491	NE	ARG	A	207	49.079	37.532	43.221	1.00	10.86	A
ATOM	1492	CZ	ARG	A	207	49.156	38.738	42.654	1.00	13.78	A
ATOM	1493	NH1	ARG	A	207	48.957	38.881	41.350	1.00	9.77	A
ATOM	1494	NH2	ARG	A	207	49.415	39.811	43.398	1.00	15.04	A
ATOM	1495	C	ARG	A	207	47.500	31.475	43.389	1.00	11.20	A
ATOM	1496	O	ARG	A	207	47.959	30.549	42.713	1.00	12.10	A
ATOM	1497	N	ILE	A	208	46.214	31.572	43.721	1.00	8.65	A
ATOM	1498	CA	ILE	A	208	45.245	30.557	43.331	1.00	8.62	A
ATOM	1499	CB	ILE	A	208	45.073	29.491	44.476	1.00	11.42	A
ATOM	1500	CG2	ILE	A	208	44.533	30.157	45.766	1.00	8.84	A
ATOM	1501	CG1	ILE	A	208	44.158	28.359	43.984	1.00	12.09	A
ATOM	1502	CD1	ILE	A	208	44.207	27.094	44.823	1.00	11.77	A
ATOM	1503	C	ILE	A	208	43.924	31.286	43.056	1.00	10.31	A
ATOM	1504	O	ILE	A	208	43.664	32.335	43.649	1.00	12.81	A
ATOM	1505	N	THR	A	209	43.098	30.776	42.145	1.00	7.78	A
ATOM	1506	CA	THR	A	209	41.825	31.470	41.864	1.00	9.01	A
ATOM	1507	CB	THR	A	209	42.055	32.610	40.849	1.00	11.48	A
ATOM	1508	OG1	THR	A	209	40.906	33.455	40.789	1.00	11.18	A
ATOM	1509	CG2	THR	A	209	42.310	32.030	39.460	1.00	12.27	A
ATOM	1510	C	THR	A	209	40.751	30.534	41.319	1.00	10.48	A
ATOM	1511	O	THR	A	209	40.978	29.326	41.215	1.00	10.85	A
ATOM	1512	N	TYR	A	210	39.577	31.087	40.997	1.00	8.58	A
ATOM	1513	CA	TYR	A	210	38.476	30.303	40.422	1.00	8.34	A
ATOM	1514	CB	TYR	A	210	37.244	30.304	41.350	1.00	4.35	A
ATOM	1515	CG	TYR	A	210	36.685	31.664	41.695	1.00	7.98	A

FIGURE 5 (continued)

25 / 46

ATOM	1516	CD1	TYR	A	210	35.656	32.240	40.927	1.00	6.11	A
ATOM	1517	CE1	TYR	A	210	35.153	33.509	41.235	1.00	7.73	A
ATOM	1518	CD2	TYR	A	210	37.188	32.386	42.778	1.00	6.57	A
ATOM	1519	CE2	TYR	A	210	36.699	33.643	43.086	1.00	5.93	A
ATOM	1520	CZ	TYR	A	210	35.687	34.203	42.313	1.00	8.47	A
ATOM	1521	OH	TYR	A	210	35.242	35.475	42.598	1.00	8.24	A
ATOM	1522	C	TYR	A	210	38.169	30.983	39.087	1.00	5.52	A
ATOM	1523	O	TYR	A	210	38.184	32.222	39.010	1.00	9.37	A
ATOM	1524	N	ILE	A	211	37.934	30.201	38.032	1.00	6.28	A
ATOM	1525	CA	ILE	A	211	37.720	30.832	36.735	1.00	7.52	A
ATOM	1526	CB	ILE	A	211	39.085	31.384	36.235	1.00	11.97	A
ATOM	1527	CG2	ILE	A	211	39.990	30.231	35.830	1.00	10.21	A
ATOM	1528	CG1	ILE	A	211	38.902	32.361	35.075	1.00	14.62	A
ATOM	1529	CD1	ILE	A	211	40.159	33.203	34.806	1.00	15.71	A
ATOM	1530	C	ILE	A	211	37.132	29.936	35.648	1.00	8.22	A
ATOM	1531	O	ILE	A	211	37.080	28.703	35.778	1.00	8.13	A
ATOM	1532	N	SER	A	212	36.634	30.590	34.602	1.00	9.06	A
ATOM	1533	CA	SER	A	212	36.140	29.913	33.394	1.00	9.98	A
ATOM	1534	CB	SER	A	212	35.984	30.934	32.256	1.00	8.45	A
ATOM	1535	OG	SER	A	212	35.637	30.283	31.037	1.00	9.53	A
ATOM	1536	C	SER	A	212	37.181	28.904	32.914	1.00	10.00	A
ATOM	1537	O	SER	A	212	38.361	29.234	32.812	1.00	7.50	A
ATOM	1538	N	PRO	A	213	36.761	27.668	32.585	1.00	8.50	A
ATOM	1539	CD	PRO	A	213	35.436	27.030	32.686	1.00	4.78	A
ATOM	1540	CA	PRO	A	213	37.781	26.728	32.117	1.00	8.39	A
ATOM	1541	CB	PRO	A	213	37.035	25.392	32.059	1.00	10.29	A
ATOM	1542	CG	PRO	A	213	35.578	25.849	31.743	1.00	9.33	A
ATOM	1543	C	PRO	A	213	38.360	27.149	30.777	1.00	10.79	A
ATOM	1544	O	PRO	A	213	39.433	26.698	30.390	1.00	10.83	A
ATOM	1545	N	ASP	A	214	37.668	28.038	30.074	1.00	5.80	A
ATOM	1546	CA	ASP	A	214	38.164	28.514	28.775	1.00	8.50	A
ATOM	1547	CB	ASP	A	214	37.033	29.175	27.997	1.00	7.35	A
ATOM	1548	CG	ASP	A	214	37.248	29.146	26.497	1.00	11.12	A
ATOM	1549	OD1	ASP	A	214	36.479	29.849	25.801	1.00	11.42	A
ATOM	1550	OD2	ASP	A	214	38.159	28.428	26.007	1.00	10.72	A
ATOM	1551	C	ASP	A	214	39.314	29.526	28.935	1.00	12.08	A
ATOM	1552	O	ASP	A	214	39.933	29.931	27.943	1.00	13.08	A
ATOM	1553	N	PHE	A	215	39.572	29.958	30.170	1.00	9.47	A
ATOM	1554	CA	PHE	A	215	40.662	30.901	30.459	1.00	9.63	A
ATOM	1555	CB	PHE	A	215	40.121	32.106	31.233	1.00	12.63	A
ATOM	1556	CG	PHE	A	215	39.375	33.081	30.402	1.00	9.86	A
ATOM	1557	CD1	PHE	A	215	39.957	34.301	30.067	1.00	11.72	A
ATOM	1558	CD2	PHE	A	215	38.074	32.812	29.986	1.00	11.34	A
ATOM	1559	CE1	PHE	A	215	39.250	35.250	29.332	1.00	11.89	A
ATOM	1560	CE2	PHE	A	215	37.357	33.759	29.245	1.00	6.37	A
ATOM	1561	CZ	PHE	A	215	37.949	34.976	28.921	1.00	13.90	A
ATOM	1562	C	PHE	A	215	41.748	30.286	31.356	1.00	13.88	A
ATOM	1563	O	PHE	A	215	42.837	30.865	31.480	1.00	12.28	A
ATOM	1564	N	ALA	A	216	41.463	29.131	31.976	1.00	9.02	A
ATOM	1565	CA	ALA	A	216	42.404	28.535	32.936	1.00	9.41	A
ATOM	1566	CB	ALA	A	216	41.705	27.432	33.753	1.00	9.18	A
ATOM	1567	C	ALA	A	216	43.727	28.007	32.406	1.00	13.18	A
ATOM	1568	O	ALA	A	216	44.679	27.844	33.178	1.00	16.82	A
ATOM	1569	N	ALA	A	217	43.790	27.719	31.106	1.00	12.39	A
ATOM	1570	CA	ALA	A	217	45.031	27.224	30.522	1.00	14.59	A
ATOM	1571	CB	ALA	A	217	45.094	25.693	30.625	1.00	15.34	A
ATOM	1572	C	ALA	A	217	45.136	27.660	29.063	1.00	16.52	A
ATOM	1573	O	ALA	A	217	44.128	27.958	28.418	1.00	14.71	A
ATOM	1574	N	PRO	A	218	46.358	27.690	28.517	1.00	18.85	A
ATOM	1575	CD	PRO	A	218	47.657	27.532	29.194	1.00	19.53	A
ATOM	1576	CA	PRO	A	218	46.533	28.101	27.111	1.00	17.17	A
ATOM	1577	CB	PRO	A	218	48.053	28.171	26.952	1.00	22.03	A
ATOM	1578	CG	PRO	A	218	48.553	28.433	28.357	1.00	24.10	A
ATOM	1579	C	PRO	A	218	45.889	27.162	26.076	1.00	17.95	A
ATOM	1580	O	PRO	A	218	45.490	27.606	24.986	1.00	20.60	A
ATOM	1581	N	SER	A	219	45.804	25.872	26.395	1.00	12.39	A
ATOM	1582	CA	SER	A	219	45.212	24.883	25.490	1.00	11.61	A
ATOM	1583	CB	SER	A	219	46.308	24.053	24.816	1.00	17.69	A
ATOM	1584	OG	SER	A	219	46.870	23.140	25.749	1.00	17.25	A
ATOM	1585	C	SER	A	219	44.341	23.942	26.324	1.00	14.52	A
ATOM	1586	O	SER	A	219	44.454	23.896	27.559	1.00	15.86	A
ATOM	1587	N	LEU	A	220	43.479	23.180	25.664	1.00	13.85	A
ATOM	1588	CA	LEU	A	220	42.614	22.250	26.389	1.00	13.63	A
ATOM	1589	CB	LEU	A	220	41.705	21.491	25.401	1.00	15.59	A
ATOM	1590	CG	LEU	A	220	40.632	22.337	24.707	1.00	16.07	A
ATOM	1591	CD1	LEU	A	220	39.908	21.517	23.646	1.00	15.58	A

FIGURE 5 (continued)

26 / 46

ATOM	1592	CD2	LEU	A	220	39.635	22.855	25.752	1.00	16.33	A
ATOM	1593	C	LEU	A	220	43.401	21.251	27.245	1.00	15.71	A
ATOM	1594	O	LEU	A	220	43.034	20.986	28.395	1.00	15.65	A
ATOM	1595	N	ALA	A	221	44.481	20.693	26.698	1.00	15.60	A
ATOM	1596	CA	ALA	A	221	45.283	19.714	27.452	1.00	18.03	A
ATOM	1597	CB	ALA	A	221	46.452	19.175	26.604	1.00	17.58	A
ATOM	1598	C	ALA	A	221	45.834	20.298	28.738	1.00	11.01	A
ATOM	1599	O	ALA	A	221	46.085	19.573	29.687	1.00	15.45	A
ATOM	1600	N	GLY	A	222	46.038	21.612	28.754	1.00	15.25	A
ATOM	1601	CA	GLY	A	222	46.561	22.267	29.947	1.00	11.71	A
ATOM	1602	C	GLY	A	222	45.641	22.101	31.144	1.00	10.72	A
ATOM	1603	O	GLY	A	222	46.105	22.139	32.280	1.00	14.13	A
ATOM	1604	N	LEU	A	223	44.340	21.938	30.914	1.00	11.19	A
ATOM	1605	CA	LEU	A	223	43.406	21.751	32.033	1.00	8.14	A
ATOM	1606	CB	LEU	A	223	41.946	21.728	31.525	1.00	9.90	A
ATOM	1607	CG	LEU	A	223	41.481	23.046	30.874	1.00	9.91	A
ATOM	1608	CD1	LEU	A	223	40.035	22.918	30.331	1.00	9.85	A
ATOM	1609	CD2	LEU	A	223	41.570	24.153	31.926	1.00	9.05	A
ATOM	1610	C	LEU	A	223	43.720	20.444	32.773	1.00	11.22	A
ATOM	1611	O	LEU	A	223	43.369	20.297	33.939	1.00	7.21	A
ATOM	1612	N	ASN	A	224	44.389	19.505	32.100	1.00	9.60	A
ATOM	1613	CA	ASN	A	224	44.742	18.231	32.727	1.00	10.35	A
ATOM	1614	CB	ASN	A	224	44.651	17.078	31.706	1.00	13.70	A
ATOM	1615	CG	ASN	A	224	43.214	16.768	31.301	1.00	15.75	A
ATOM	1616	OD1	ASN	A	224	42.347	16.610	32.146	1.00	21.72	A
ATOM	1617	ND2	ASN	A	224	42.968	16.666	30.012	1.00	14.86	A
ATOM	1618	C	ASN	A	224	46.138	18.239	33.359	1.00	12.93	A
ATOM	1619	O	ASN	A	224	46.580	17.226	33.898	1.00	14.86	A
ATOM	1620	N	ASP	A	225	46.833	19.370	33.308	1.00	8.74	A
ATOM	1621	CA	ASP	A	225	48.163	19.437	33.932	1.00	12.69	A
ATOM	1622	CB	ASP	A	225	49.031	20.467	33.199	1.00	11.40	A
ATOM	1623	CG	ASP	A	225	50.402	20.654	33.843	1.00	15.89	A
ATOM	1624	OD1	ASP	A	225	50.673	20.076	34.922	1.00	14.10	A
ATOM	1625	OD2	ASP	A	225	51.211	21.401	33.261	1.00	16.19	A
ATOM	1626	C	ASP	A	225	47.960	19.844	35.398	1.00	13.53	A
ATOM	1627	O	ASP	A	225	47.776	21.016	35.691	1.00	10.79	A
ATOM	1628	N	ALA	A	226	48.035	18.882	36.317	1.00	10.49	A
ATOM	1629	CA	ALA	A	226	47.792	19.178	37.720	1.00	9.18	A
ATOM	1630	CB	ALA	A	226	47.424	17.889	38.478	1.00	13.20	A
ATOM	1631	C	ALA	A	226	48.881	19.939	38.461	1.00	12.23	A
ATOM	1632	O	ALA	A	226	48.773	20.144	39.678	1.00	13.15	A
ATOM	1633	N	THR	A	227	49.935	20.347	37.762	1.00	10.64	A
ATOM	1634	CA	THR	A	227	50.955	21.148	38.426	1.00	10.50	A
ATOM	1635	CB	THR	A	227	52.405	20.854	37.917	1.00	15.63	A
ATOM	1636	OG1	THR	A	227	52.541	21.287	36.561	1.00	13.88	A
ATOM	1637	CG2	THR	A	227	52.718	19.374	38.009	1.00	16.59	A
ATOM	1638	C	THR	A	227	50.620	22.628	38.154	1.00	9.17	A
ATOM	1639	O	THR	A	227	51.320	23.509	38.626	1.00	10.52	A
ATOM	1640	N	LYS	A	228	49.530	22.876	37.414	1.00	9.27	A
ATOM	1641	CA	LYS	A	228	49.079	24.226	37.069	1.00	12.05	A
ATOM	1642	CB	LYS	A	228	49.378	24.511	35.594	1.00	15.38	A
ATOM	1643	CG	LYS	A	228	50.877	24.607	35.272	1.00	22.71	A
ATOM	1644	CD	LYS	A	228	51.125	24.652	33.758	1.00	20.66	A
ATOM	1645	CE	LYS	A	228	52.613	24.720	33.447	1.00	26.84	A
ATOM	1646	NZ	LYS	A	228	53.205	25.974	33.986	1.00	37.16	A
ATOM	1647	C	LYS	A	228	47.576	24.453	37.313	1.00	8.78	A
ATOM	1648	O	LYS	A	228	47.153	25.574	37.634	1.00	9.99	A
ATOM	1649	N	VAL	A	229	46.777	23.407	37.100	1.00	9.98	A
ATOM	1650	CA	VAL	A	229	45.327	23.465	37.282	1.00	6.71	A
ATOM	1651	CB	VAL	A	229	44.611	23.300	35.939	1.00	8.87	A
ATOM	1652	CG1	VAL	A	229	43.082	23.303	36.150	1.00	10.77	A
ATOM	1653	CG2	VAL	A	229	45.019	24.468	34.988	1.00	10.90	A
ATOM	1654	C	VAL	A	229	44.913	22.339	38.245	1.00	10.51	A
ATOM	1655	O	VAL	A	229	45.107	21.154	37.967	1.00	8.04	A
ATOM	1656	N	ALA	A	230	44.343	22.706	39.383	1.00	10.29	A
ATOM	1657	CA	ALA	A	230	43.985	21.696	40.387	1.00	8.30	A
ATOM	1658	CB	ALA	A	230	43.612	22.380	41.677	1.00	10.71	A
ATOM	1659	C	ALA	A	230	42.900	20.691	40.064	1.00	12.18	A
ATOM	1660	O	ALA	A	230	41.884	21.020	39.435	1.00	12.58	A
ATOM	1661	N	ARG	A	231	43.120	19.452	40.501	1.00	8.23	A
ATOM	1662	CA	ARG	A	231	42.080	18.436	40.382	1.00	8.98	A
ATOM	1663	CB	ARG	A	231	42.656	17.021	40.495	1.00	11.67	A
ATOM	1664	CG	ARG	A	231	43.433	16.581	39.265	1.00	14.58	A
ATOM	1665	CD	ARG	A	231	44.130	15.244	39.487	1.00	18.76	A
ATOM	1666	NE	ARG	A	231	44.972	14.941	38.336	1.00	19.63	A
ATOM	1667	CZ	ARG	A	231	45.931	14.029	38.331	1.00	26.24	A

FIGURE 5 (continued)

27 / 46

ATOM	1668	NH1	ARG	A	231	46.184	13.312	39.426	1.00	22.17	A
ATOM	1669	NH2	ARG	A	231	46.649	13.848	37.228	1.00	31.31	A
ATOM	1670	C	ARG	A	231	41.271	18.738	41.632	1.00	8.66	A
ATOM	1671	O	ARG	A	231	41.801	19.332	42.582	1.00	13.24	A
ATOM	1672	N	THR	A	232	39.997	18.371	41.640	1.00	9.11	A
ATOM	1673	CA	THR	A	232	39.180	18.607	42.822	1.00	11.84	A
ATOM	1674	CB	THR	A	232	38.236	19.820	42.623	1.00	13.64	A
ATOM	1675	OG1	THR	A	232	39.017	21.004	42.384	1.00	17.60	A
ATOM	1676	CG2	THR	A	232	37.382	20.025	43.883	1.00	14.43	A
ATOM	1677	C	THR	A	232	38.357	17.351	43.071	1.00	9.12	A
ATOM	1678	O	THR	A	232	37.869	16.747	42.118	1.00	13.13	A
ATOM	1679	N	GLY	A	233	38.240	16.934	44.332	1.00	9.55	A
ATOM	1680	CA	GLY	A	233	37.466	15.739	44.636	1.00	13.57	A
ATOM	1681	C	GLY	A	233	38.197	14.616	45.364	1.00	14.09	A
ATOM	1682	O	GLY	A	233	37.634	13.556	45.591	1.00	16.30	A
ATOM	1683	N	LYS	A	234	39.460	14.831	45.706	1.00	14.67	A
ATOM	1684	CA	LYS	A	234	40.226	13.834	46.438	1.00	15.04	A
ATOM	1685	CB	LYS	A	234	41.577	14.442	46.830	1.00	13.37	A
ATOM	1686	CG	LYS	A	234	42.483	13.576	47.688	1.00	14.40	A
ATOM	1687	CD	LYS	A	234	43.807	14.314	47.968	1.00	17.84	A
ATOM	1688	CE	LYS	A	234	43.594	15.567	48.839	1.00	15.78	A
ATOM	1689	NZ	LYS	A	234	44.766	16.501	48.832	1.00	12.74	A
ATOM	1690	C	LYS	A	234	39.450	13.411	47.697	1.00	17.96	A
ATOM	1691	O	LYS	A	234	38.826	14.240	48.369	1.00	13.45	A
ATOM	1692	N	GLY	A	235	39.489	12.124	48.031	1.00	15.80	A
ATOM	1693	CA	GLY	A	235	38.785	11.694	49.223	1.00	15.51	A
ATOM	1694	C	GLY	A	235	38.764	10.191	49.402	1.00	19.91	A
ATOM	1695	O	GLY	A	235	39.586	9.472	48.825	1.00	21.77	A
ATOM	1696	N	SER	A	236	37.811	9.731	50.204	1.00	21.18	A
ATOM	1697	CA	SER	A	236	37.624	8.311	50.489	1.00	24.63	A
ATOM	1698	CB	SER	A	236	38.018	8.004	51.929	1.00	25.33	A
ATOM	1699	OG	SER	A	236	39.359	8.397	52.161	1.00	33.33	A
ATOM	1700	C	SER	A	236	36.159	7.969	50.291	1.00	26.45	A
ATOM	1701	O	SER	A	236	35.282	8.624	50.855	1.00	27.89	A
ATOM	1702	N	SER	A	237	35.891	6.947	49.488	1.00	22.58	A
ATOM	1703	CA	SER	A	237	34.522	6.520	49.238	1.00	23.79	A
ATOM	1704	CB	SER	A	237	34.123	6.799	47.786	1.00	25.37	A
ATOM	1705	OG	SER	A	237	34.019	8.197	47.578	1.00	38.24	A
ATOM	1706	C	SER	A	237	34.429	5.036	49.514	1.00	21.92	A
ATOM	1707	O	SER	A	237	35.244	4.267	49.009	1.00	20.25	A
ATOM	1708	N	SER	A	238	33.423	4.640	50.295	1.00	25.14	A
ATOM	1709	CA	SER	A	238	33.233	3.236	50.662	1.00	24.45	A
ATOM	1710	CB	SER	A	238	32.716	2.427	49.471	1.00	27.22	A
ATOM	1711	OG	SER	A	238	31.371	2.785	49.163	1.00	39.35	A
ATOM	1712	C	SER	A	238	34.559	2.670	51.159	1.00	23.39	A
ATOM	1713	O	SER	A	238	34.961	1.557	50.809	1.00	24.29	A
ATOM	1714	N	GLY	A	239	35.249	3.468	51.966	1.00	24.50	A
ATOM	1715	CA	GLY	A	239	36.519	3.040	52.524	1.00	25.11	A
ATOM	1716	C	GLY	A	239	37.705	2.973	51.584	1.00	28.40	A
ATOM	1717	O	GLY	A	239	38.755	2.452	51.969	1.00	28.03	A
ATOM	1718	N	GLY	A	240	37.563	3.495	50.365	1.00	21.59	A
ATOM	1719	CA	GLY	A	240	38.677	3.459	49.431	1.00	26.05	A
ATOM	1720	C	GLY	A	240	39.082	4.858	48.984	1.00	24.32	A
ATOM	1721	O	GLY	A	240	38.218	5.685	48.714	1.00	23.70	A
ATOM	1722	N	GLY	A	241	40.386	5.121	48.920	1.00	21.49	A
ATOM	1723	CA	GLY	A	241	40.873	6.422	48.500	1.00	27.38	A
ATOM	1724	C	GLY	A	241	40.495	6.715	47.058	1.00	28.81	A
ATOM	1725	O	GLY	A	241	40.585	5.840	46.200	1.00	28.58	A
ATOM	1726	N	ALA	A	242	40.057	7.939	46.784	1.00	24.66	A
ATOM	1727	CA	ALA	A	242	39.663	8.303	45.434	1.00	22.08	A
ATOM	1728	CB	ALA	A	242	38.159	8.527	45.367	1.00	25.95	A
ATOM	1729	C	ALA	A	242	40.385	9.573	45.043	1.00	22.46	A
ATOM	1730	O	ALA	A	242	40.541	10.472	45.869	1.00	16.67	A
ATOM	1731	N	GLU	A	243	40.813	9.647	43.785	1.00	16.24	A
ATOM	1732	CA	GLU	A	243	41.502	10.830	43.289	1.00	18.78	A
ATOM	1733	CB	GLU	A	243	42.444	10.473	42.132	1.00	23.30	A
ATOM	1734	CG	GLU	A	243	43.643	9.624	42.499	1.00	31.37	A
ATOM	1735	CD	GLU	A	243	44.658	9.584	41.368	1.00	37.64	A
ATOM	1736	OE1	GLU	A	243	44.234	9.507	40.195	1.00	38.59	A
ATOM	1737	OE2	GLU	A	243	45.876	9.628	41.644	1.00	41.94	A
ATOM	1738	C	GLU	A	243	40.469	11.817	42.757	1.00	15.80	A
ATOM	1739	O	GLU	A	243	39.417	11.406	42.285	1.00	17.65	A
ATOM	1740	N	GLY	A	244	40.765	13.111	42.827	1.00	15.34	A
ATOM	1741	CA	GLY	A	244	39.832	14.101	42.286	1.00	16.23	A
ATOM	1742	C	GLY	A	244	39.994	14.161	40.770	1.00	16.48	A
ATOM	1743	O	GLY	A	244	40.894	13.528	40.228	1.00	14.37	A

FIGURE 5 (continued)

28 / 46

ATOM	1744	N	LYS	A	245	39.148	14.939	40.096	1.00	14.99	A
ATOM	1745	CA	LYS	A	245	39.186	15.079	38.632	1.00	14.88	A
ATOM	1746	CB	LYS	A	245	37.792	14.795	38.060	1.00	13.06	A
ATOM	1747	CG	LYS	A	245	37.294	13.363	38.289	1.00	22.95	A
ATOM	1748	CD	LYS	A	245	38.174	12.353	37.540	1.00	27.44	A
ATOM	1749	CE	LYS	A	245	37.596	10.939	37.643	1.00	27.64	A
ATOM	1750	NZ	LYS	A	245	37.298	10.599	39.063	1.00	36.34	A
ATOM	1751	C	LYS	A	245	39.617	16.471	38.165	1.00	13.81	A
ATOM	1752	O	LYS	A	245	39.580	17.431	38.932	1.00	10.66	A
ATOM	1753	N	SER	A	246	40.022	16.572	36.902	1.00	14.72	A
ATOM	1754	CA	SER	A	246	40.405	17.856	36.344	1.00	11.87	A
ATOM	1755	CB	SER	A	246	41.299	17.687	35.104	1.00	12.31	A
ATOM	1756	OG	SER	A	246	40.515	17.215	34.011	1.00	9.67	A
ATOM	1757	C	SER	A	246	39.095	18.500	35.913	1.00	10.79	A
ATOM	1758	O	SER	A	246	38.076	17.815	35.735	1.00	10.08	A
ATOM	1759	N	PRO	A	247	39.114	19.825	35.698	1.00	10.98	A
ATOM	1760	CD	PRO	A	247	40.243	20.747	35.947	1.00	7.03	A
ATOM	1761	CA	PRO	A	247	37.909	20.545	35.275	1.00	9.29	A
ATOM	1762	CB	PRO	A	247	38.210	21.988	35.692	1.00	7.19	A
ATOM	1763	CG	PRO	A	247	39.737	22.094	35.385	1.00	9.12	A
ATOM	1764	C	PRO	A	247	37.632	20.416	33.765	1.00	9.99	A
ATOM	1765	O	PRO	A	247	36.865	21.197	33.222	1.00	11.54	A
ATOM	1766	N	ALA	A	248	38.253	19.449	33.083	1.00	9.23	A
ATOM	1767	CA	ALA	A	248	37.992	19.278	31.638	1.00	12.63	A
ATOM	1768	CB	ALA	A	248	38.832	18.097	31.069	1.00	10.35	A
ATOM	1769	C	ALA	A	248	36.487	19.021	31.431	1.00	15.07	A
ATOM	1770	O	ALA	A	248	35.838	18.390	32.278	1.00	11.60	A
ATOM	1771	N	ALA	A	249	35.935	19.497	30.311	1.00	12.95	A
ATOM	1772	CA	ALA	A	249	34.498	19.332	30.037	1.00	11.90	A
ATOM	1773	CB	ALA	A	249	34.141	19.886	28.633	1.00	12.61	A
ATOM	1774	C	ALA	A	249	34.037	17.890	30.149	1.00	15.30	A
ATOM	1775	O	ALA	A	249	32.953	17.617	30.666	1.00	14.63	A
ATOM	1776	N	ALA	A	250	34.845	16.949	29.672	1.00	14.76	A
ATOM	1777	CA	ALA	A	250	34.426	15.542	29.769	1.00	18.41	A
ATOM	1778	CB	ALA	A	250	35.486	14.623	29.168	1.00	15.53	A
ATOM	1779	C	ALA	A	250	34.118	15.102	31.200	1.00	15.76	A
ATOM	1780	O	ALA	A	250	33.366	14.154	31.410	1.00	14.59	A
ATOM	1781	N	ASN	A	251	34.677	15.785	32.190	1.00	14.82	A
ATOM	1782	CA	ASN	A	251	34.433	15.380	33.575	1.00	13.85	A
ATOM	1783	CB	ASN	A	251	35.665	15.696	34.441	1.00	12.26	A
ATOM	1784	CG	ASN	A	251	36.880	14.885	34.022	1.00	14.85	A
ATOM	1785	OD1	ASN	A	251	36.755	13.712	33.653	1.00	14.23	A
ATOM	1786	ND2	ASN	A	251	38.056	15.487	34.091	1.00	13.09	A
ATOM	1787	C	ASN	A	251	33.168	15.968	34.210	1.00	16.10	A
ATOM	1788	O	ASN	A	251	32.877	15.686	35.357	1.00	14.41	A
ATOM	1789	N	SER	A	252	32.431	16.806	33.482	1.00	13.25	A
ATOM	1790	CA	SER	A	252	31.191	17.346	34.039	1.00	10.81	A
ATOM	1791	CB	SER	A	252	31.262	18.868	34.209	1.00	22.32	A
ATOM	1792	OG	SER	A	252	31.266	19.536	32.953	1.00	23.58	A
ATOM	1793	C	SER	A	252	30.027	16.982	33.101	1.00	11.68	A
ATOM	1794	O	SER	A	252	28.862	17.077	33.479	1.00	12.18	A
ATOM	1795	N	SER	A	253	30.365	16.501	31.904	1.00	11.74	A
ATOM	1796	CA	SER	A	253	29.367	16.138	30.918	1.00	10.64	A
ATOM	1797	CB	SER	A	253	30.048	15.572	29.665	1.00	18.81	A
ATOM	1798	OG	SER	A	253	29.052	15.263	28.704	1.00	27.87	A
ATOM	1799	C	SER	A	253	28.294	15.139	31.382	1.00	15.51	A
ATOM	1800	O	SER	A	253	27.112	15.319	31.102	1.00	11.29	A
ATOM	1801	N	ALA	A	254	28.692	14.080	32.081	1.00	12.85	A
ATOM	1802	CA	ALA	A	254	27.700	13.084	32.525	1.00	14.75	A
ATOM	1803	CB	ALA	A	254	28.423	11.868	33.216	1.00	13.94	A
ATOM	1804	C	ALA	A	254	26.656	13.667	33.472	1.00	14.13	A
ATOM	1805	O	ALA	A	254	25.457	13.394	33.342	1.00	14.40	A
ATOM	1806	N	ALA	A	255	27.111	14.457	34.441	1.00	11.77	A
ATOM	1807	CA	ALA	A	255	26.205	15.070	35.401	1.00	13.30	A
ATOM	1808	CB	ALA	A	255	27.009	15.838	36.460	1.00	12.60	A
ATOM	1809	C	ALA	A	255	25.223	16.017	34.698	1.00	15.34	A
ATOM	1810	O	ALA	A	255	24.068	16.162	35.113	1.00	14.03	A
ATOM	1811	N	ILE	A	256	25.684	16.680	33.644	1.00	13.10	A
ATOM	1812	CA	ILE	A	256	24.812	17.599	32.920	1.00	14.09	A
ATOM	1813	CB	ILE	A	256	25.614	18.445	31.900	1.00	11.60	A
ATOM	1814	CG2	ILE	A	256	24.655	19.233	30.987	1.00	13.12	A
ATOM	1815	CG1	ILE	A	256	26.577	19.378	32.657	1.00	8.87	A
ATOM	1816	CD1	ILE	A	256	25.878	20.335	33.703	1.00	6.00	A
ATOM	1817	C	ILE	A	256	23.716	16.813	32.195	1.00	12.88	A
ATOM	1818	O	ILE	A	256	22.569	17.268	32.118	1.00	12.14	A
ATOM	1819	N	SER	A	257	24.069	15.639	31.678	1.00	12.01	A

FIGURE 5 (continued)

29 / 46

ATOM	1820	CA	SER	A	257	23.105	14.793	30.960	1.00	17.17	A
ATOM	1821	CB	SER	A	257	23.773	13.529	30.418	1.00	20.37	A
ATOM	1822	OG	SER	A	257	24.331	13.802	29.157	1.00	27.40	A
ATOM	1823	C	SER	A	257	21.886	14.359	31.750	1.00	21.46	A
ATOM	1824	O	SER	A	257	20.885	13.975	31.161	1.00	25.54	A
ATOM	1825	N	VAL	A	258	21.949	14.417	33.070	1.00	18.37	A
ATOM	1826	CA	VAL	A	258	20.803	13.983	33.849	1.00	22.61	A
ATOM	1827	CB	VAL	A	258	21.230	13.049	34.996	1.00	23.45	A
ATOM	1828	CG1	VAL	A	258	22.055	11.887	34.443	1.00	28.56	A
ATOM	1829	CG2	VAL	A	258	22.004	13.831	36.041	1.00	29.85	A
ATOM	1830	C	VAL	A	258	20.002	15.133	34.436	1.00	20.13	A
ATOM	1831	O	VAL	A	258	19.056	14.907	35.193	1.00	19.13	A
ATOM	1832	N	VAL	A	259	20.367	16.365	34.092	1.00	17.82	A
ATOM	1833	CA	VAL	A	259	19.628	17.503	34.621	1.00	12.10	A
ATOM	1834	CB	VAL	A	259	20.345	18.816	34.305	1.00	9.61	A
ATOM	1835	CG1	VAL	A	259	19.448	20.009	34.655	1.00	9.95	A
ATOM	1836	CG2	VAL	A	259	21.661	18.870	35.110	1.00	9.60	A
ATOM	1837	C	VAL	A	259	18.257	17.470	33.946	1.00	10.93	A
ATOM	1838	O	VAL	A	259	18.154	17.543	32.719	1.00	12.34	A
ATOM	1839	N	PRO	A	260	17.185	17.372	34.746	1.00	12.49	A
ATOM	1840	CD	PRO	A	260	17.178	17.349	36.227	1.00	15.54	A
ATOM	1841	CA	PRO	A	260	15.823	17.321	34.204	1.00	12.14	A
ATOM	1842	CB	PRO	A	260	14.992	16.881	35.415	1.00	18.68	A
ATOM	1843	CG	PRO	A	260	15.705	17.553	36.556	1.00	20.90	A
ATOM	1844	C	PRO	A	260	15.326	18.629	33.592	1.00	13.33	A
ATOM	1845	O	PRO	A	260	15.719	19.704	34.025	1.00	11.59	A
ATOM	1846	N	LEU	A	261	14.462	18.517	32.583	1.00	10.89	A
ATOM	1847	CA	LEU	A	261	13.906	19.697	31.899	1.00	14.89	A
ATOM	1848	CB	LEU	A	261	13.190	19.272	30.612	1.00	14.36	A
ATOM	1849	CG	LEU	A	261	14.033	18.724	29.470	1.00	23.33	A
ATOM	1850	CD1	LEU	A	261	13.132	18.115	28.388	1.00	17.91	A
ATOM	1851	CD2	LEU	A	261	14.860	19.854	28.927	1.00	21.86	A
ATOM	1852	C	LEU	A	261	12.868	20.354	32.782	1.00	14.14	A
ATOM	1853	O	LEU	A	261	12.313	19.715	33.667	1.00	13.00	A
ATOM	1854	N	PRO	A	262	12.598	21.646	32.570	1.00	16.56	A
ATOM	1855	CD	PRO	A	262	13.154	22.620	31.613	1.00	18.10	A
ATOM	1856	CA	PRO	A	262	11.576	22.260	33.421	1.00	16.86	A
ATOM	1857	CB	PRO	A	262	11.753	23.752	33.137	1.00	16.37	A
ATOM	1858	CG	PRO	A	262	12.147	23.764	31.698	1.00	22.55	A
ATOM	1859	C	PRO	A	262	10.239	21.709	32.911	1.00	14.68	A
ATOM	1860	O	PRO	A	262	10.136	21.357	31.743	1.00	14.32	A
ATOM	1861	N	ALA	A	263	9.234	21.605	33.776	1.00	13.42	A
ATOM	1862	CA	ALA	A	263	7.943	21.085	33.344	1.00	16.60	A
ATOM	1863	CB	ALA	A	263	6.994	20.952	34.539	1.00	20.02	A
ATOM	1864	C	ALA	A	263	7.343	22.011	32.292	1.00	16.04	A
ATOM	1865	O	ALA	A	263	7.480	23.235	32.377	1.00	14.70	A
ATOM	1866	N	ALA	A	264	6.664	21.426	31.309	1.00	15.42	A
ATOM	1867	CA	ALA	A	264	6.050	22.206	30.239	1.00	12.74	A
ATOM	1868	CB	ALA	A	264	5.248	21.287	29.308	1.00	19.88	A
ATOM	1869	C	ALA	A	264	5.149	23.329	30.747	1.00	15.82	A
ATOM	1870	O	ALA	A	264	5.247	24.461	30.264	1.00	17.34	A
ATOM	1871	N	ALA	A	265	4.284	23.037	31.721	1.00	13.78	A
ATOM	1872	CA	ALA	A	265	3.370	24.071	32.242	1.00	15.17	A
ATOM	1873	CB	ALA	A	265	2.464	23.478	33.363	1.00	15.42	A
ATOM	1874	C	ALA	A	265	4.057	25.333	32.772	1.00	15.06	A
ATOM	1875	O	ALA	A	265	3.437	26.398	32.838	1.00	13.78	A
ATOM	1876	N	ASN	A	266	5.320	25.212	33.175	1.00	13.85	A
ATOM	1877	CA	ASN	A	266	6.057	26.343	33.733	1.00	12.11	A
ATOM	1878	CB	ASN	A	266	6.987	25.895	34.873	1.00	13.94	A
ATOM	1879	CG	ASN	A	266	6.253	25.239	36.028	1.00	23.25	A
ATOM	1880	OD1	ASN	A	266	5.175	25.676	36.425	1.00	21.92	A
ATOM	1881	ND2	ASN	A	266	6.856	24.200	36.592	1.00	19.37	A
ATOM	1882	C	ASN	A	266	6.969	27.039	32.730	1.00	12.06	A
ATOM	1883	O	ASN	A	266	7.662	27.965	33.100	1.00	13.88	A
ATOM	1884	N	ARG	A	267	6.980	26.600	31.483	1.00	10.11	A
ATOM	1885	CA	ARG	A	267	7.933	27.162	30.534	1.00	12.44	A
ATOM	1886	CB	ARG	A	267	8.029	26.254	29.306	1.00	10.57	A
ATOM	1887	CG	ARG	A	267	8.746	24.945	29.675	1.00	12.04	A
ATOM	1888	CD	ARG	A	267	8.892	23.924	28.540	1.00	9.95	A
ATOM	1889	NE	ARG	A	267	9.275	22.637	29.124	1.00	14.76	A
ATOM	1890	CZ	ARG	A	267	9.533	21.530	28.439	1.00	14.94	A
ATOM	1891	NH1	ARG	A	267	9.477	21.543	27.118	1.00	16.59	A
ATOM	1892	NH2	ARG	A	267	9.782	20.387	29.084	1.00	12.17	A
ATOM	1893	C	ARG	A	267	7.785	28.629	30.168	1.00	13.15	A
ATOM	1894	O	ARG	A	267	8.658	29.207	29.505	1.00	13.32	A
ATOM	1895	N	GLY	A	268	6.711	29.240	30.663	1.00	11.13	A

FIGURE 5 (continued)

30 / 46

ATOM	1896	CA	GLY	A	268	6.491	30.653	30.439	1.00	13.33	A
ATOM	1897	C	GLY	A	268	7.212	31.457	31.507	1.00	13.92	A
ATOM	1898	O	GLY	A	268	7.219	32.679	31.452	1.00	14.39	A
ATOM	1899	N	ASP	A	269	7.804	30.767	32.486	1.00	11.00	A
ATOM	1900	CA	ASP	A	269	8.554	31.398	33.594	1.00	14.58	A
ATOM	1901	CB	ASP	A	269	8.233	30.665	34.914	1.00	13.17	A
ATOM	1902	CG	ASP	A	269	8.943	31.263	36.117	1.00	16.24	A
ATOM	1903	OD1	ASP	A	269	9.767	32.179	35.944	1.00	17.40	A
ATOM	1904	OD2	ASP	A	269	8.667	30.804	37.244	1.00	19.44	A
ATOM	1905	C	ASP	A	269	10.064	31.290	33.303	1.00	10.72	A
ATOM	1906	O	ASP	A	269	10.616	30.196	33.348	1.00	11.39	A
ATOM	1907	N	PRO	A	270	10.742	32.417	33.010	1.00	11.52	A
ATOM	1908	CD	PRO	A	270	10.217	33.796	32.924	1.00	11.48	A
ATOM	1909	CA	PRO	A	270	12.184	32.394	32.709	1.00	10.44	A
ATOM	1910	CB	PRO	A	270	12.523	33.867	32.491	1.00	11.04	A
ATOM	1911	CG	PRO	A	270	11.225	34.465	32.026	1.00	13.30	A
ATOM	1912	C	PRO	A	270	13.042	31.786	33.793	1.00	12.77	A
ATOM	1913	O	PRO	A	270	14.097	31.243	33.521	1.00	10.58	A
ATOM	1914	N	ASN	A	271	12.578	31.870	35.032	1.00	11.41	A
ATOM	1915	CA	ASN	A	271	13.337	31.332	36.145	1.00	11.19	A
ATOM	1916	CB	ASN	A	271	12.660	31.729	37.463	1.00	14.43	A
ATOM	1917	CG	ASN	A	271	13.533	31.434	38.683	1.00	22.14	A
ATOM	1918	OD1	ASN	A	271	14.734	31.726	38.696	1.00	16.89	A
ATOM	1919	ND2	ASN	A	271	12.934	30.854	39.703	1.00	16.43	A
ATOM	1920	C	ASN	A	271	13.545	29.816	36.090	1.00	16.21	A
ATOM	1921	O	ASN	A	271	14.595	29.319	36.510	1.00	15.74	A
ATOM	1922	N	VAL	A	272	12.574	29.065	35.575	1.00	10.21	A
ATOM	1923	CA	VAL	A	272	12.749	27.613	35.547	1.00	11.32	A
ATOM	1924	CB	VAL	A	272	11.378	26.849	35.440	1.00	13.38	A
ATOM	1925	CG1	VAL	A	272	10.450	27.297	36.548	1.00	14.31	A
ATOM	1926	CG2	VAL	A	272	10.759	27.074	34.078	1.00	11.03	A
ATOM	1927	C	VAL	A	272	13.651	27.086	34.434	1.00	12.71	A
ATOM	1928	O	VAL	A	272	14.028	25.907	34.459	1.00	10.89	A
ATOM	1929	N	TRP	A	273	13.991	27.930	33.461	1.00	7.57	A
ATOM	1930	CA	TRP	A	273	14.862	27.465	32.366	1.00	7.83	A
ATOM	1931	CB	TRP	A	273	14.741	28.403	31.150	1.00	7.08	A
ATOM	1932	CG	TRP	A	273	13.496	28.126	30.364	1.00	10.87	A
ATOM	1933	CD2	TRP	A	273	13.359	27.161	29.325	1.00	9.80	A
ATOM	1934	CE2	TRP	A	273	12.020	27.228	28.860	1.00	9.21	A
ATOM	1935	CE3	TRP	A	273	14.241	26.240	28.732	1.00	10.74	A
ATOM	1936	CD1	TRP	A	273	12.271	28.728	30.500	1.00	7.74	A
ATOM	1937	NE1	TRP	A	273	11.375	28.192	29.590	1.00	12.31	A
ATOM	1938	CZ2	TRP	A	273	11.545	26.412	27.838	1.00	10.97	A
ATOM	1939	CZ3	TRP	A	273	13.764	25.428	27.700	1.00	10.91	A
ATOM	1940	CH2	TRP	A	273	12.427	25.522	27.267	1.00	14.13	A
ATOM	1941	C	TRP	A	273	16.338	27.311	32.755	1.00	9.26	A
ATOM	1942	O	TRP	A	273	17.119	26.663	32.042	1.00	9.73	A
ATOM	1943	N	THR	A	274	16.736	27.893	33.880	1.00	8.74	A
ATOM	1944	CA	THR	A	274	18.123	27.769	34.281	1.00	11.71	A
ATOM	1945	CB	THR	A	274	18.759	29.147	34.542	1.00	12.87	A
ATOM	1946	OG1	THR	A	274	18.701	29.940	33.334	1.00	16.61	A
ATOM	1947	CG2	THR	A	274	20.240	28.973	34.959	1.00	9.96	A
ATOM	1948	C	THR	A	274	18.271	26.918	35.535	1.00	10.53	A
ATOM	1949	O	THR	A	274	18.020	27.378	36.645	1.00	11.96	A
ATOM	1950	N	PRO	A	275	18.673	25.657	35.373	1.00	11.80	A
ATOM	1951	CD	PRO	A	275	18.885	24.916	34.119	1.00	13.30	A
ATOM	1952	CA	PRO	A	275	18.841	24.782	36.543	1.00	11.14	A
ATOM	1953	CB	PRO	A	275	19.180	23.424	35.921	1.00	15.21	A
ATOM	1954	CG	PRO	A	275	18.600	23.506	34.528	1.00	15.39	A
ATOM	1955	C	PRO	A	275	20.004	25.253	37.445	1.00	12.51	A
ATOM	1956	O	PRO	A	275	21.007	25.723	36.950	1.00	12.15	A
ATOM	1957	N	VAL	A	276	19.869	25.148	38.764	1.00	9.91	A
ATOM	1958	CA	VAL	A	276	20.999	25.502	39.615	1.00	10.08	A
ATOM	1959	CB	VAL	A	276	20.738	26.762	40.478	1.00	15.02	A
ATOM	1960	CG1	VAL	A	276	20.534	27.990	39.568	1.00	16.57	A
ATOM	1961	CG2	VAL	A	276	19.551	26.543	41.388	1.00	17.45	A
ATOM	1962	C	VAL	A	276	21.236	24.293	40.500	1.00	12.75	A
ATOM	1963	O	VAL	A	276	20.315	23.498	40.743	1.00	7.21	A
ATOM	1964	N	PHE	A	277	22.472	24.149	40.969	1.00	13.38	A
ATOM	1965	CA	PHE	A	277	22.848	23.017	41.798	1.00	12.43	A
ATOM	1966	CB	PHE	A	277	24.231	22.491	41.373	1.00	8.49	A
ATOM	1967	CG	PHE	A	277	24.229	21.828	40.017	1.00	8.19	A
ATOM	1968	CD1	PHE	A	277	24.404	22.568	38.858	1.00	9.76	A
ATOM	1969	CD2	PHE	A	277	23.999	20.461	39.909	1.00	8.15	A
ATOM	1970	CE1	PHE	A	277	24.350	21.934	37.585	1.00	13.41	A
ATOM	1971	CE2	PHE	A	277	23.938	19.825	38.654	1.00	13.62	A

FIGURE 5 (continued)

31 / 46

ATOM	1972	CZ	PHE	A	277	24.114	20.555	37.499	1.00	8.74	A
ATOM	1973	C	PHE	A	277	22.848	23.377	43.272	1.00	12.19	A
ATOM	1974	O	PHE	A	277	22.892	24.553	43.634	1.00	12.80	A
ATOM	1975	N	GLY	A	278	22.781	22.356	44.116	1.00	12.01	A
ATOM	1976	CA	GLY	A	278	22.767	22.601	45.547	1.00	10.29	A
ATOM	1977	C	GLY	A	278	23.113	21.342	46.309	1.00	9.39	A
ATOM	1978	O	GLY	A	278	23.379	20.302	45.704	1.00	12.45	A
ATOM	1979	N	ALA	A	279	23.087	21.414	47.637	1.00	11.15	A
ATOM	1980	CA	ALA	A	279	23.436	20.246	48.450	1.00	14.32	A
ATOM	1981	CB	ALA	A	279	23.362	20.604	49.930	1.00	16.91	A
ATOM	1982	C	ALA	A	279	22.542	19.029	48.157	1.00	20.18	A
ATOM	1983	O	ALA	A	279	23.038	17.896	48.017	1.00	18.69	A
ATOM	1984	N	VAL	A	280	21.238	19.262	48.040	1.00	14.35	A
ATOM	1985	CA	VAL	A	280	20.302	18.176	47.796	1.00	19.81	A
ATOM	1986	CB	VAL	A	280	19.500	17.847	49.076	1.00	23.28	A
ATOM	1987	CG1	VAL	A	280	20.457	17.579	50.225	1.00	23.97	A
ATOM	1988	CG2	VAL	A	280	18.603	18.992	49.436	1.00	21.87	A
ATOM	1989	C	VAL	A	280	19.311	18.483	46.686	1.00	20.63	A
ATOM	1990	O	VAL	A	280	19.004	19.635	46.407	1.00	21.63	A
ATOM	1991	N	THR	A	281	18.812	17.436	46.055	1.00	20.03	A
ATOM	1992	CA	THR	A	281	17.838	17.599	44.982	1.00	19.32	A
ATOM	1993	CB	THR	A	281	17.732	16.327	44.136	1.00	20.70	A
ATOM	1994	OG1	THR	A	281	18.989	16.096	43.493	1.00	24.83	A
ATOM	1995	CG2	THR	A	281	16.637	16.473	43.062	1.00	20.23	A
ATOM	1996	C	THR	A	281	16.500	17.882	45.618	1.00	24.45	A
ATOM	1997	O	THR	A	281	16.073	17.159	46.520	1.00	22.56	A
ATOM	1998	N	GLY	A	282	15.854	18.949	45.164	1.00	22.37	A
ATOM	1999	CA	GLY	A	282	14.564	19.316	45.706	1.00	26.62	A
ATOM	2000	C	GLY	A	282	14.183	20.735	45.343	1.00	31.11	A
ATOM	2001	O	GLY	A	282	15.048	21.603	45.206	1.00	27.54	A
ATOM	2002	N	GLY	A	283	12.883	20.971	45.181	1.00	32.42	A
ATOM	2003	CA	GLY	A	283	12.401	22.301	44.855	1.00	30.56	A
ATOM	2004	C	GLY	A	283	13.051	22.950	43.654	1.00	30.47	A
ATOM	2005	O	GLY	A	283	13.307	24.154	43.666	1.00	33.57	A
ATOM	2006	N	GLY	A	284	13.298	22.171	42.607	1.00	26.82	A
ATOM	2007	CA	GLY	A	284	13.925	22.723	41.415	1.00	26.01	A
ATOM	2008	C	GLY	A	284	15.450	22.687	41.439	1.00	26.04	A
ATOM	2009	O	GLY	A	284	16.115	22.822	40.406	1.00	25.82	A
ATOM	2010	N	VAL	A	285	16.022	22.521	42.622	1.00	19.46	A
ATOM	2011	CA	VAL	A	285	17.467	22.461	42.722	1.00	19.85	A
ATOM	2012	CB	VAL	A	285	17.903	22.894	44.135	1.00	19.90	A
ATOM	2013	CG1	VAL	A	285	19.389	22.673	44.319	1.00	16.38	A
ATOM	2014	CG2	VAL	A	285	17.521	24.376	44.360	1.00	20.29	A
ATOM	2015	C	VAL	A	285	17.958	21.037	42.428	1.00	18.72	A
ATOM	2016	O	VAL	A	285	17.298	20.055	42.794	1.00	18.51	A
ATOM	2017	N	VAL	A	286	19.103	20.932	41.755	1.00	14.01	A
ATOM	2018	CA	VAL	A	286	19.706	19.645	41.423	1.00	16.59	A
ATOM	2019	CB	VAL	A	286	20.200	19.625	39.964	1.00	14.25	A
ATOM	2020	CG1	VAL	A	286	20.729	18.254	39.623	1.00	19.16	A
ATOM	2021	CG2	VAL	A	286	19.068	19.997	39.036	1.00	20.67	A
ATOM	2022	C	VAL	A	286	20.917	19.416	42.325	1.00	17.27	A
ATOM	2023	O	VAL	A	286	21.757	20.302	42.484	1.00	13.49	A
ATOM	2024	N	ALA	A	287	21.041	18.229	42.896	1.00	15.01	A
ATOM	2025	CA	ALA	A	287	22.188	18.000	43.778	1.00	17.78	A
ATOM	2026	CB	ALA	A	287	22.039	16.649	44.527	1.00	16.62	A
ATOM	2027	C	ALA	A	287	23.483	18.011	42.999	1.00	12.88	A
ATOM	2028	O	ALA	A	287	23.520	17.533	41.854	1.00	10.29	A
ATOM	2029	N	TYR	A	288	24.538	18.576	43.603	1.00	11.08	A
ATOM	2030	CA	TYR	A	288	25.867	18.554	42.979	1.00	8.88	A
ATOM	2031	CB	TYR	A	288	26.877	19.297	43.862	1.00	12.41	A
ATOM	2032	CG	TYR	A	288	26.891	20.803	43.649	1.00	9.59	A
ATOM	2033	CD1	TYR	A	288	26.329	21.677	44.589	1.00	8.82	A
ATOM	2034	CE1	TYR	A	288	26.320	23.086	44.382	1.00	10.11	A
ATOM	2035	CD2	TYR	A	288	27.463	21.356	42.491	1.00	10.87	A
ATOM	2036	CE2	TYR	A	288	27.464	22.744	42.275	1.00	6.63	A
ATOM	2037	CZ	TYR	A	288	26.883	23.601	43.223	1.00	7.60	A
ATOM	2038	OH	TYR	A	288	26.842	24.960	42.960	1.00	7.46	A
ATOM	2039	C	TYR	A	288	26.263	17.061	42.851	1.00	12.67	A
ATOM	2040	O	TYR	A	288	25.989	16.265	43.750	1.00	10.55	A
ATOM	2041	N	PRO	A	289	26.929	16.672	41.746	1.00	12.61	A
ATOM	2042	CD	PRO	A	289	27.338	17.560	40.625	1.00	13.50	A
ATOM	2043	CA	PRO	A	289	27.346	15.280	41.495	1.00	12.99	A
ATOM	2044	CB	PRO	A	289	27.863	15.328	40.051	1.00	15.51	A
ATOM	2045	CG	PRO	A	289	28.424	16.734	39.920	1.00	10.53	A
ATOM	2046	C	PRO	A	289	28.366	14.644	42.439	1.00	17.46	A
ATOM	2047	O	PRO	A	289	29.342	15.282	42.835	1.00	15.29	A

FIGURE 5 (continued)

32 / 46

ATOM	2048	N	ASP	A	290	28.149	13.372	42.782	1.00	16.57	A
ATOM	2049	CA	ASP	A	290	29.092	12.691	43.652	1.00	20.97	A
ATOM	2050	CB	ASP	A	290	28.360	11.751	44.628	1.00	25.52	A
ATOM	2051	CG	ASP	A	290	27.489	10.723	43.929	1.00	34.64	A
ATOM	2052	OD1	ASP	A	290	26.599	10.146	44.604	1.00	38.07	A
ATOM	2053	OD2	ASP	A	290	27.693	10.478	42.716	1.00	39.24	A
ATOM	2054	C	ASP	A	290	30.154	11.952	42.824	1.00	21.23	A
ATOM	2055	O	ASP	A	290	30.990	11.231	43.362	1.00	21.11	A
ATOM	2056	N	SER	A	291	30.136	12.152	41.509	1.00	14.24	A
ATOM	2057	CA	SER	A	291	31.143	11.538	40.645	1.00	16.28	A
ATOM	2058	CB	SER	A	291	30.592	10.290	39.925	1.00	16.14	A
ATOM	2059	OG	SER	A	291	29.549	10.625	39.031	1.00	22.17	A
ATOM	2060	C	SER	A	291	31.555	12.609	39.643	1.00	14.75	A
ATOM	2061	O	SER	A	291	30.842	13.605	39.493	1.00	13.50	A
ATOM	2062	N	GLY	A	292	32.692	12.419	38.971	1.00	13.79	A
ATOM	2063	CA	GLY	A	292	33.181	13.423	38.019	1.00	14.60	A
ATOM	2064	C	GLY	A	292	33.713	14.688	38.707	1.00	11.05	A
ATOM	2065	O	GLY	A	292	33.964	14.669	39.909	1.00	14.10	A
ATOM	2066	N	TYR	A	293	33.904	15.779	37.955	1.00	10.56	A
ATOM	2067	CA	TYR	A	293	34.380	17.049	38.529	1.00	9.23	A
ATOM	2068	CB	TYR	A	293	34.838	18.014	37.443	1.00	10.30	A
ATOM	2069	CG	TYR	A	293	35.535	19.229	38.012	1.00	11.13	A
ATOM	2070	CD1	TYR	A	293	36.829	19.138	38.526	1.00	7.85	A
ATOM	2071	CE1	TYR	A	293	37.482	20.269	39.049	1.00	8.64	A
ATOM	2072	CD2	TYR	A	293	34.900	20.470	38.038	1.00	11.82	A
ATOM	2073	CE2	TYR	A	293	35.547	21.601	38.554	1.00	11.43	A
ATOM	2074	CZ	TYR	A	293	36.839	21.488	39.052	1.00	8.40	A
ATOM	2075	OH	TYR	A	293	37.488	22.625	39.496	1.00	8.49	A
ATOM	2076	C	TYR	A	293	33.183	17.645	39.252	1.00	9.71	A
ATOM	2077	O	TYR	A	293	32.142	17.834	38.657	1.00	12.02	A
ATOM	2078	N	PRO	A	294	33.347	18.021	40.531	1.00	12.25	A
ATOM	2079	CD	PRO	A	294	34.575	17.923	41.350	1.00	12.44	A
ATOM	2080	CA	PRO	A	294	32.229	18.559	41.302	1.00	14.24	A
ATOM	2081	CB	PRO	A	294	32.644	18.263	42.748	1.00	12.15	A
ATOM	2082	CG	PRO	A	294	34.132	18.499	42.712	1.00	15.49	A
ATOM	2083	C	PRO	A	294	31.682	19.963	41.133	1.00	13.85	A
ATOM	2084	O	PRO	A	294	30.511	20.171	41.429	1.00	11.37	A
ATOM	2085	N	ILE	A	295	32.476	20.907	40.628	1.00	10.88	A
ATOM	2086	CA	ILE	A	295	31.990	22.280	40.510	1.00	9.12	A
ATOM	2087	CB	ILE	A	295	33.062	23.301	40.934	1.00	10.07	A
ATOM	2088	CG2	ILE	A	295	32.375	24.666	41.232	1.00	10.52	A
ATOM	2089	CG1	ILE	A	295	33.733	22.853	42.236	1.00	12.06	A
ATOM	2090	CD1	ILE	A	295	34.841	23.801	42.703	1.00	12.46	A
ATOM	2091	C	ILE	A	295	31.564	22.574	39.087	1.00	12.87	A
ATOM	2092	O	ILE	A	295	32.397	22.660	38.182	1.00	10.57	A
ATOM	2093	N	LEU	A	296	30.257	22.743	38.902	1.00	10.82	A
ATOM	2094	CA	LEU	A	296	29.703	22.951	37.570	1.00	8.61	A
ATOM	2095	CB	LEU	A	296	29.370	21.578	36.949	1.00	9.63	A
ATOM	2096	CG	LEU	A	296	28.032	20.884	37.276	1.00	7.75	A
ATOM	2097	CD1	LEU	A	296	27.971	19.517	36.572	1.00	11.60	A
ATOM	2098	CD2	LEU	A	296	27.852	20.690	38.784	1.00	10.20	A
ATOM	2099	C	LEU	A	296	28.461	23.828	37.612	1.00	7.00	A
ATOM	2100	O	LEU	A	296	27.945	24.137	38.690	1.00	11.47	A
ATOM	2101	N	GLY	A	297	27.988	24.236	36.436	1.00	8.98	A
ATOM	2102	CA	GLY	A	297	26.812	25.093	36.353	1.00	8.75	A
ATOM	2103	C	GLY	A	297	26.503	25.452	34.906	1.00	14.03	A
ATOM	2104	O	GLY	A	297	27.128	24.917	33.979	1.00	9.23	A
ATOM	2105	N	PHE	A	298	25.544	26.353	34.700	1.00	7.40	A
ATOM	2106	CA	PHE	A	298	25.177	26.758	33.350	1.00	7.84	A
ATOM	2107	CB	PHE	A	298	23.666	26.550	33.105	1.00	6.30	A
ATOM	2108	CG	PHE	A	298	23.249	25.102	32.984	1.00	10.10	A
ATOM	2109	CD1	PHE	A	298	22.775	24.398	34.094	1.00	9.62	A
ATOM	2110	CD2	PHE	A	298	23.356	24.444	31.763	1.00	8.37	A
ATOM	2111	CE1	PHE	A	298	22.414	23.038	33.988	1.00	13.84	A
ATOM	2112	CE2	PHE	A	298	23.005	23.087	31.630	1.00	7.19	A
ATOM	2113	CZ	PHE	A	298	22.533	22.379	32.747	1.00	12.00	A
ATOM	2114	C	PHE	A	298	25.469	28.235	33.145	1.00	10.22	A
ATOM	2115	O	PHE	A	298	25.431	29.007	34.114	1.00	9.27	A
ATOM	2116	N	THR	A	299	25.811	28.615	31.910	1.00	7.04	A
ATOM	2117	CA	THR	A	299	25.961	30.029	31.594	1.00	8.99	A
ATOM	2118	CB	THR	A	299	27.319	30.414	30.975	1.00	12.65	A
ATOM	2119	OG1	THR	A	299	27.293	31.818	30.682	1.00	10.67	A
ATOM	2120	CG2	THR	A	299	27.616	29.617	29.740	1.00	12.18	A
ATOM	2121	C	THR	A	299	24.798	30.220	30.616	1.00	8.12	A
ATOM	2122	O	THR	A	299	24.482	29.325	29.810	1.00	9.48	A
ATOM	2123	N	ASP	A	300	24.173	31.392	30.677	1.00	8.49	A

FIGURE 5 (continued)

33 / 46

ATOM	2124	CA	ASP	A	300	22.930	31.636	29.950	1.00	10.66	A
ATOM	2125	CB	ASP	A	300	21.849	31.816	31.023	1.00	8.23	A
ATOM	2126	CG	ASP	A	300	22.055	30.877	32.193	1.00	14.11	A
ATOM	2127	OD1	ASP	A	300	22.141	29.660	31.928	1.00	8.23	A
ATOM	2128	OD2	ASP	A	300	22.149	31.341	33.373	1.00	15.65	A
ATOM	2129	C	ASP	A	300	22.828	32.790	28.975	1.00	10.65	A
ATOM	2130	O	ASP	A	300	23.690	33.669	28.931	1.00	8.49	A
ATOM	2131	N	LEU	A	301	21.740	32.765	28.202	1.00	8.77	A
ATOM	2132	CA	LEU	A	301	21.407	33.819	27.246	1.00	10.49	A
ATOM	2133	CB	LEU	A	301	21.121	33.226	25.850	1.00	10.57	A
ATOM	2134	CG	LEU	A	301	22.189	32.371	25.157	1.00	17.61	A
ATOM	2135	CD1	LEU	A	301	21.699	31.951	23.775	1.00	16.46	A
ATOM	2136	CD2	LEU	A	301	23.456	33.151	25.057	1.00	12.96	A
ATOM	2137	C	LEU	A	301	20.128	34.533	27.689	1.00	7.85	A
ATOM	2138	O	LEU	A	301	19.179	33.889	28.127	1.00	7.63	A
ATOM	2139	N	ILE	A	302	20.101	35.855	27.564	1.00	8.91	A
ATOM	2140	CA	ILE	A	302	18.897	36.614	27.879	1.00	7.82	A
ATOM	2141	CB	ILE	A	302	19.146	37.648	29.000	1.00	10.36	A
ATOM	2142	CG2	ILE	A	302	17.848	38.429	29.261	1.00	12.51	A
ATOM	2143	CG1	ILE	A	302	19.588	36.918	30.287	1.00	8.81	A
ATOM	2144	CD1	ILE	A	302	20.089	37.867	31.411	1.00	7.82	A
ATOM	2145	C	ILE	A	302	18.517	37.368	26.602	1.00	9.48	A
ATOM	2146	O	ILE	A	302	19.320	38.158	26.096	1.00	8.44	A
ATOM	2147	N	PHE	A	303	17.311	37.120	26.081	1.00	8.80	A
ATOM	2148	CA	PHE	A	303	16.843	37.786	24.854	1.00	8.37	A
ATOM	2149	CB	PHE	A	303	16.751	36.821	23.651	1.00	7.07	A
ATOM	2150	CG	PHE	A	303	18.054	36.583	22.944	1.00	8.30	A
ATOM	2151	CD1	PHE	A	303	19.027	35.770	23.500	1.00	8.48	A
ATOM	2152	CD2	PHE	A	303	18.316	37.205	21.725	1.00	7.08	A
ATOM	2153	CE1	PHE	A	303	20.265	35.582	22.851	1.00	7.30	A
ATOM	2154	CE2	PHE	A	303	19.559	37.023	21.065	1.00	9.28	A
ATOM	2155	CZ	PHE	A	303	20.528	36.210	21.637	1.00	11.64	A
ATOM	2156	C	PHE	A	303	15.437	38.305	25.032	1.00	9.03	A
ATOM	2157	O	PHE	A	303	14.797	38.052	26.031	1.00	9.30	A
ATOM	2158	N	SER	A	304	14.947	39.002	24.014	1.00	7.56	A
ATOM	2159	CA	SER	A	304	13.566	39.465	24.044	1.00	9.72	A
ATOM	2160	CB	SER	A	304	13.470	40.870	23.444	1.00	11.08	A
ATOM	2161	OG	SER	A	304	12.117	41.291	23.498	1.00	10.08	A
ATOM	2162	C	SER	A	304	12.707	38.530	23.170	1.00	6.80	A
ATOM	2163	O	SER	A	304	13.198	38.018	22.162	1.00	10.90	A
ATOM	2164	N	GLU	A	305	11.451	38.293	23.534	1.00	8.14	A
ATOM	2165	CA	GLU	A	305	10.605	37.482	22.655	1.00	11.11	A
ATOM	2166	CB	GLU	A	305	9.268	37.125	23.316	1.00	10.66	A
ATOM	2167	CG	GLU	A	305	8.447	36.161	22.439	1.00	11.71	A
ATOM	2168	CD	GLU	A	305	7.073	35.820	22.985	1.00	12.77	A
ATOM	2169	OE1	GLU	A	305	6.767	36.154	24.147	1.00	14.12	A
ATOM	2170	OE2	GLU	A	305	6.288	35.192	22.228	1.00	16.70	A
ATOM	2171	C	GLU	A	305	10.305	38.329	21.399	1.00	15.34	A
ATOM	2172	O	GLU	A	305	10.154	37.800	20.283	1.00	10.74	A
ATOM	2173	N	CYS	A	306	10.239	39.649	21.574	1.00	11.86	A
ATOM	2174	CA	CYS	A	306	9.889	40.534	20.450	1.00	12.96	A
ATOM	2175	C	CYS	A	306	10.859	41.666	20.140	1.00	14.14	A
ATOM	2176	O	CYS	A	306	11.434	42.270	21.046	1.00	11.98	A
ATOM	2177	CB	CYS	A	306	8.531	41.185	20.726	1.00	11.40	A
ATOM	2178	SG	CYS	A	306	7.188	40.111	21.313	1.00	15.63	A
ATOM	2179	N	TYR	A	307	11.017	41.956	18.854	1.00	12.82	A
ATOM	2180	CA	TYR	A	307	11.872	43.060	18.397	1.00	10.85	A
ATOM	2181	CB	TYR	A	307	13.143	42.533	17.712	1.00	8.88	A
ATOM	2182	CG	TYR	A	307	14.066	41.850	18.703	1.00	13.96	A
ATOM	2183	CD1	TYR	A	307	13.902	40.499	19.020	1.00	13.44	A
ATOM	2184	CE1	TYR	A	307	14.683	39.882	20.020	1.00	13.43	A
ATOM	2185	CD2	TYR	A	307	15.035	42.579	19.401	1.00	11.32	A
ATOM	2186	CE2	TYR	A	307	15.821	41.972	20.410	1.00	11.99	A
ATOM	2187	CZ	TYR	A	307	15.637	40.625	20.712	1.00	12.10	A
ATOM	2188	OH	TYR	A	307	16.379	40.019	21.724	1.00	12.32	A
ATOM	2189	C	TYR	A	307	11.056	43.908	17.424	1.00	13.04	A
ATOM	2190	O	TYR	A	307	10.318	43.370	16.588	1.00	11.71	A
ATOM	2191	N	ALA	A	308	11.161	45.229	17.546	1.00	13.47	A
ATOM	2192	CA	ALA	A	308	10.420	46.123	16.660	1.00	19.16	A
ATOM	2193	CB	ALA	A	308	10.623	47.583	17.116	1.00	19.39	A
ATOM	2194	C	ALA	A	308	10.827	45.960	15.176	1.00	16.58	A
ATOM	2195	O	ALA	A	308	9.990	46.011	14.290	1.00	15.94	A
ATOM	2196	N	ASN	A	309	12.109	45.752	14.919	1.00	16.56	A
ATOM	2197	CA	ASN	A	309	12.621	45.602	13.565	1.00	15.71	A
ATOM	2198	CB	ASN	A	309	14.084	46.052	13.558	1.00	11.74	A
ATOM	2199	CG	ASN	A	309	14.704	46.002	12.183	1.00	20.62	A

FIGURE 5 (continued)

34 / 46

ATOM	2200	OD1	ASN	A	309	15.130	44.946	11.713	1.00	17.26	A
ATOM	2201	ND2	ASN	A	309	14.741	47.153	11.517	1.00	13.84	A
ATOM	2202	C	ASN	A	309	12.493	44.142	13.066	1.00	16.39	A
ATOM	2203	O	ASN	A	309	13.031	43.221	13.678	1.00	11.54	A
ATOM	2204	N	ALA	A	310	11.806	43.942	11.941	1.00	12.69	A
ATOM	2205	CA	ALA	A	310	11.583	42.584	11.430	1.00	16.06	A
ATOM	2206	CB	ALA	A	310	10.564	42.618	10.281	1.00	16.44	A
ATOM	2207	C	ALA	A	310	12.836	41.828	10.997	1.00	14.76	A
ATOM	2208	O	ALA	A	310	12.907	40.599	11.128	1.00	15.90	A
ATOM	2209	N	THR	A	311	13.827	42.546	10.485	1.00	13.61	A
ATOM	2210	CA	THR	A	311	15.074	41.922	10.069	1.00	14.28	A
ATOM	2211	CB	THR	A	311	15.949	42.927	9.314	1.00	15.47	A
ATOM	2212	OG1	THR	A	311	15.284	43.307	8.097	1.00	18.10	A
ATOM	2213	CG2	THR	A	311	17.291	42.322	8.977	1.00	16.40	A
ATOM	2214	C	THR	A	311	15.813	41.407	11.324	1.00	15.00	A
ATOM	2215	O	THR	A	311	16.371	40.313	11.318	1.00	12.29	A
ATOM	2216	N	GLN	A	312	15.798	42.180	12.409	1.00	13.08	A
ATOM	2217	CA	GLN	A	312	16.477	41.717	13.623	1.00	12.35	A
ATOM	2218	CB	GLN	A	312	16.545	42.827	14.682	1.00	10.08	A
ATOM	2219	CG	GLN	A	312	17.501	43.960	14.273	1.00	7.89	A
ATOM	2220	CD	GLN	A	312	17.696	44.997	15.377	1.00	13.93	A
ATOM	2221	OE1	GLN	A	312	16.897	45.087	16.311	1.00	14.28	A
ATOM	2222	NE2	GLN	A	312	18.743	45.799	15.255	1.00	16.18	A
ATOM	2223	C	GLN	A	312	15.768	40.486	14.191	1.00	11.19	A
ATOM	2224	O	GLN	A	312	16.418	39.537	14.639	1.00	14.09	A
ATOM	2225	N	THR	A	313	14.439	40.507	14.189	1.00	9.72	A
ATOM	2226	CA	THR	A	313	13.670	39.363	14.685	1.00	8.88	A
ATOM	2227	CB	THR	A	313	12.149	39.541	14.449	1.00	13.95	A
ATOM	2228	OG1	THR	A	313	11.660	40.660	15.197	1.00	14.46	A
ATOM	2229	CG2	THR	A	313	11.398	38.288	14.882	1.00	12.76	A
ATOM	2230	C	THR	A	313	14.108	38.096	13.935	1.00	10.80	A
ATOM	2231	O	THR	A	313	14.318	37.042	14.538	1.00	11.41	A
ATOM	2232	N	GLY	A	314	14.218	38.204	12.615	1.00	11.55	A
ATOM	2233	CA	GLY	A	314	14.628	37.067	11.810	1.00	12.96	A
ATOM	2234	C	GLY	A	314	16.060	36.638	12.090	1.00	10.31	A
ATOM	2235	O	GLY	A	314	16.370	35.439	12.111	1.00	11.80	A
ATOM	2236	N	GLN	A	315	16.952	37.603	12.291	1.00	10.00	A
ATOM	2237	CA	GLN	A	315	18.360	37.280	12.586	1.00	10.98	A
ATOM	2238	CB	GLN	A	315	19.219	38.542	12.512	1.00	12.34	A
ATOM	2239	CG	GLN	A	315	19.286	39.069	11.071	1.00	13.86	A
ATOM	2240	CD	GLN	A	315	20.014	40.385	10.958	1.00	16.05	A
ATOM	2241	OE1	GLN	A	315	19.868	41.254	11.818	1.00	15.65	A
ATOM	2242	NE2	GLN	A	315	20.787	40.552	9.880	1.00	15.34	A
ATOM	2243	C	GLN	A	315	18.518	36.613	13.952	1.00	11.33	A
ATOM	2244	O	GLN	A	315	19.385	35.743	14.136	1.00	12.86	A
ATOM	2245	N	VAL	A	316	17.677	37.006	14.909	1.00	11.99	A
ATOM	2246	CA	VAL	A	316	17.719	36.389	16.238	1.00	11.29	A
ATOM	2247	CB	VAL	A	316	16.803	37.131	17.251	1.00	12.97	A
ATOM	2248	CG1	VAL	A	316	16.658	36.292	18.541	1.00	12.95	A
ATOM	2249	CG2	VAL	A	316	17.401	38.493	17.602	1.00	11.75	A
ATOM	2250	C	VAL	A	316	17.232	34.929	16.092	1.00	13.11	A
ATOM	2251	O	VAL	A	316	17.813	33.996	16.667	1.00	12.64	A
ATOM	2252	N	ARG	A	317	16.164	34.723	15.327	1.00	9.04	A
ATOM	2253	CA	ARG	A	317	15.672	33.364	15.115	1.00	12.87	A
ATOM	2254	CB	ARG	A	317	14.348	33.372	14.303	1.00	14.06	A
ATOM	2255	CG	ARG	A	317	13.148	33.951	15.076	1.00	13.07	A
ATOM	2256	CD	ARG	A	317	11.823	33.964	14.243	1.00	14.93	A
ATOM	2257	NE	ARG	A	317	11.520	32.611	13.765	1.00	14.57	A
ATOM	2258	CZ	ARG	A	317	10.894	31.677	14.480	1.00	10.03	A
ATOM	2259	NH1	ARG	A	317	10.470	31.934	15.704	1.00	9.62	A
ATOM	2260	NH2	ARG	A	317	10.730	30.461	13.983	1.00	13.56	A
ATOM	2261	C	ARG	A	317	16.730	32.491	14.434	1.00	12.01	A
ATOM	2262	O	ARG	A	317	16.879	31.320	14.783	1.00	12.09	A
ATOM	2263	N	ASN	A	318	17.462	33.033	13.464	1.00	11.68	A
ATOM	2264	CA	ASN	A	318	18.503	32.246	12.796	1.00	13.18	A
ATOM	2265	CB	ASN	A	318	19.123	33.028	11.629	1.00	11.52	A
ATOM	2266	CG	ASN	A	318	18.145	33.249	10.500	1.00	15.15	A
ATOM	2267	OD1	ASN	A	318	17.140	32.557	10.402	1.00	13.70	A
ATOM	2268	ND2	ASN	A	318	18.438	34.211	9.638	1.00	17.31	A
ATOM	2269	C	ASN	A	318	19.613	31.841	13.771	1.00	12.19	A
ATOM	2270	O	ASN	A	318	20.207	30.753	13.658	1.00	9.01	A
ATOM	2271	N	PHE	A	319	19.904	32.715	14.733	1.00	10.68	A
ATOM	2272	CA	PHE	A	319	20.936	32.376	15.707	1.00	9.90	A
ATOM	2273	CB	PHE	A	319	21.274	33.577	16.584	1.00	7.66	A
ATOM	2274	CG	PHE	A	319	22.105	33.212	17.794	1.00	10.09	A
ATOM	2275	CD1	PHE	A	319	23.351	32.644	17.631	1.00	6.01	A

FIGURE 5 (continued)

35 / 46

ATOM	2276	CD2	PHE	A	319	21.593	33.356	19.087	1.00	10.54	A
ATOM	2277	CE1	PHE	A	319	24.102	32.203	18.738	1.00	12.72	A
ATOM	2278	CE2	PHE	A	319	22.333	32.919	20.212	1.00	15.07	A
ATOM	2279	CZ	PHE	A	319	23.589	32.338	20.027	1.00	12.59	A
ATOM	2280	C	PHE	A	319	20.449	31.222	16.587	1.00	10.27	A
ATOM	2281	O	PHE	A	319	21.203	30.282	16.868	1.00	12.47	A
ATOM	2282	N	PHE	A	320	19.188	31.275	17.013	1.00	10.21	A
ATOM	2283	CA	PHE	A	320	18.649	30.213	17.860	1.00	10.79	A
ATOM	2284	CB	PHE	A	320	17.247	30.581	18.363	1.00	9.11	A
ATOM	2285	CG	PHE	A	320	17.246	31.285	19.698	1.00	7.96	A
ATOM	2286	CD1	PHE	A	320	16.762	30.642	20.833	1.00	9.52	A
ATOM	2287	CD2	PHE	A	320	17.723	32.583	19.822	1.00	12.60	A
ATOM	2288	CE1	PHE	A	320	16.750	31.282	22.082	1.00	6.69	A
ATOM	2289	CE2	PHE	A	320	17.712	33.244	21.075	1.00	9.45	A
ATOM	2290	CZ	PHE	A	320	17.220	32.579	22.209	1.00	8.89	A
ATOM	2291	C	PHE	A	320	18.598	28.912	17.089	1.00	7.76	A
ATOM	2292	O	PHE	A	320	18.856	27.838	17.634	1.00	9.90	A
ATOM	2293	N	THR	A	321	18.274	29.013	15.801	1.00	8.04	A
ATOM	2294	CA	THR	A	321	18.199	27.829	14.950	1.00	6.79	A
ATOM	2295	CB	THR	A	321	17.687	28.224	13.551	1.00	7.01	A
ATOM	2296	OG1	THR	A	321	16.334	28.695	13.691	1.00	11.25	A
ATOM	2297	CG2	THR	A	321	17.731	27.032	12.573	1.00	9.32	A
ATOM	2298	C	THR	A	321	19.535	27.128	14.872	1.00	11.09	A
ATOM	2299	O	THR	A	321	19.594	25.896	14.823	1.00	10.46	A
ATOM	2300	N	LYS	A	322	20.617	27.904	14.873	1.00	8.41	A
ATOM	2301	CA	LYS	A	322	21.950	27.319	14.849	1.00	8.00	A
ATOM	2302	CB	LYS	A	322	22.970	28.329	14.299	1.00	6.38	A
ATOM	2303	CG	LYS	A	322	24.410	27.805	14.359	1.00	10.15	A
ATOM	2304	CD	LYS	A	322	25.396	28.712	13.615	1.00	8.08	A
ATOM	2305	CE	LYS	A	322	26.665	27.922	13.317	1.00	11.78	A
ATOM	2306	NZ	LYS	A	322	27.577	28.702	12.437	1.00	18.79	A
ATOM	2307	C	LYS	A	322	22.415	26.857	16.242	1.00	9.52	A
ATOM	2308	O	LYS	A	322	22.864	25.711	16.425	1.00	9.02	A
ATOM	2309	N	HIS	A	323	22.289	27.735	17.231	1.00	10.06	A
ATOM	2310	CA	HIS	A	323	22.793	27.420	18.569	1.00	9.00	A
ATOM	2311	CB	HIS	A	323	22.710	28.677	19.469	1.00	7.78	A
ATOM	2312	CG	HIS	A	323	23.655	28.657	20.637	1.00	9.56	A
ATOM	2313	CD2	HIS	A	323	23.426	28.762	21.970	1.00	9.53	A
ATOM	2314	ND1	HIS	A	323	25.028	28.560	20.494	1.00	7.88	A
ATOM	2315	CE1	HIS	A	323	25.602	28.615	21.683	1.00	9.47	A
ATOM	2316	NE2	HIS	A	323	24.653	28.736	22.598	1.00	12.97	A
ATOM	2317	C	HIS	A	323	22.082	26.230	19.222	1.00	9.52	A
ATOM	2318	O	HIS	A	323	22.687	25.507	20.019	1.00	8.65	A
ATOM	2319	N	TYR	A	324	20.808	26.034	18.877	1.00	9.61	A
ATOM	2320	CA	TYR	A	324	20.024	24.911	19.427	1.00	10.38	A
ATOM	2321	CB	TYR	A	324	18.767	25.434	20.149	1.00	6.95	A
ATOM	2322	CG	TYR	A	324	19.137	26.376	21.277	1.00	7.33	A
ATOM	2323	CD1	TYR	A	324	19.195	27.752	21.072	1.00	5.99	A
ATOM	2324	CE1	TYR	A	324	19.656	28.618	22.097	1.00	8.99	A
ATOM	2325	CD2	TYR	A	324	19.533	25.882	22.513	1.00	7.61	A
ATOM	2326	CE2	TYR	A	324	19.994	26.731	23.525	1.00	5.98	A
ATOM	2327	CZ	TYR	A	324	20.052	28.094	23.303	1.00	7.54	A
ATOM	2328	OH	TYR	A	324	20.547	28.926	24.294	1.00	7.56	A
ATOM	2329	C	TYR	A	324	19.627	23.893	18.338	1.00	7.02	A
ATOM	2330	O	TYR	A	324	18.677	23.118	18.498	1.00	10.94	A
ATOM	2331	N	GLY	A	325	20.387	23.868	17.254	1.00	7.94	A
ATOM	2332	CA	GLY	A	325	20.064	22.938	16.181	1.00	7.51	A
ATOM	2333	C	GLY	A	325	20.514	21.493	16.386	1.00	12.01	A
ATOM	2334	O	GLY	A	325	21.492	21.227	17.097	1.00	10.59	A
ATOM	2335	N	THR	A	326	19.788	20.564	15.752	1.00	8.75	A
ATOM	2336	CA	THR	A	326	20.113	19.132	15.790	1.00	10.25	A
ATOM	2337	CB	THR	A	326	19.005	18.311	15.135	1.00	9.46	A
ATOM	2338	OG1	THR	A	326	17.759	18.707	15.708	1.00	10.73	A
ATOM	2339	CG2	THR	A	326	19.212	16.788	15.369	1.00	7.67	A
ATOM	2340	C	THR	A	326	21.432	18.937	15.038	1.00	9.78	A
ATOM	2341	O	THR	A	326	22.278	18.131	15.452	1.00	10.90	A
ATOM	2342	N	SER	A	327	21.614	19.688	13.953	1.00	12.37	A
ATOM	2343	CA	SER	A	327	22.858	19.666	13.176	1.00	11.58	A
ATOM	2344	CB	SER	A	327	22.743	18.752	11.935	1.00	14.65	A
ATOM	2345	OG	SER	A	327	21.725	19.192	11.051	1.00	10.13	A
ATOM	2346	C	SER	A	327	23.158	21.118	12.764	1.00	10.87	A
ATOM	2347	O	SER	A	327	22.419	22.031	13.149	1.00	9.05	A
ATOM	2348	N	ALA	A	328	24.228	21.331	12.000	1.00	11.22	A
ATOM	2349	CA	ALA	A	328	24.637	22.690	11.567	1.00	10.30	A
ATOM	2350	CB	ALA	A	328	23.682	23.234	10.518	1.00	12.01	A
ATOM	2351	C	ALA	A	328	24.602	23.592	12.790	1.00	11.88	A

FIGURE 5 (continued)

TITLE: NOVEL PHOSPHATE-BINDING PROTEIN, PHARMACEUTICAL COMPOSITIONS CONTAINING SAME AND USE THEREOF

36 / 46

ATOM	2352	O	ALA	A	328	24.046	24.674	12.742	1.00	13.69	A
ATOM	2353	N	ASN	A	329	25.197	23.140	13.887	1.00	11.26	A
ATOM	2354	CA	ASN	A	329	25.150	23.910	15.123	1.00	10.51	A
ATOM	2355	CB	ASN	A	329	24.422	23.083	16.205	1.00	8.81	A
ATOM	2356	CG	ASN	A	329	25.132	21.771	16.536	1.00	9.32	A
ATOM	2357	OD1	ASN	A	329	26.352	21.717	16.573	1.00	11.49	A
ATOM	2358	ND2	ASN	A	329	24.360	20.714	16.792	1.00	10.75	A
ATOM	2359	C	ASN	A	329	26.526	24.402	15.604	1.00	12.21	A
ATOM	2360	O	ASN	A	329	27.515	24.381	14.849	1.00	9.35	A
ATOM	2361	N	ASP	A	330	26.586	24.863	16.851	1.00	10.38	A
ATOM	2362	CA	ASP	A	330	27.837	25.386	17.412	1.00	9.41	A
ATOM	2363	CB	ASP	A	330	27.575	26.677	18.208	1.00	10.91	A
ATOM	2364	CG	ASP	A	330	27.239	27.852	17.331	1.00	13.71	A
ATOM	2365	OD1	ASP	A	330	26.333	28.653	17.720	1.00	14.93	A
ATOM	2366	OD2	ASP	A	330	27.880	27.981	16.261	1.00	10.16	A
ATOM	2367	C	ASP	A	330	28.536	24.416	18.346	1.00	10.31	A
ATOM	2368	O	ASP	A	330	29.484	24.809	19.029	1.00	8.29	A
ATOM	2369	N	ASN	A	331	28.111	23.153	18.363	1.00	8.79	A
ATOM	2370	CA	ASN	A	331	28.698	22.217	19.311	1.00	10.91	A
ATOM	2371	CB	ASN	A	331	27.942	20.869	19.267	1.00	11.40	A
ATOM	2372	CG	ASN	A	331	26.579	20.924	19.989	1.00	15.36	A
ATOM	2373	OD1	ASN	A	331	25.926	19.893	20.194	1.00	12.09	A
ATOM	2374	ND2	ASN	A	331	26.156	22.115	20.372	1.00	9.71	A
ATOM	2375	C	ASN	A	331	30.220	22.012	19.218	1.00	12.28	A
ATOM	2376	O	ASN	A	331	30.877	21.866	20.255	1.00	12.57	A
ATOM	2377	N	ALA	A	332	30.795	22.001	18.012	1.00	10.00	A
ATOM	2378	CA	ALA	A	332	32.252	21.842	17.903	1.00	12.41	A
ATOM	2379	CB	ALA	A	332	32.677	21.733	16.445	1.00	12.06	A
ATOM	2380	C	ALA	A	332	32.964	23.028	18.548	1.00	8.53	A
ATOM	2381	O	ALA	A	332	33.973	22.872	19.247	1.00	11.75	A
ATOM	2382	N	ALA	A	333	32.447	24.216	18.297	1.00	9.64	A
ATOM	2383	CA	ALA	A	333	33.057	25.422	18.858	1.00	10.83	A
ATOM	2384	CB	ALA	A	333	32.424	26.655	18.223	1.00	9.42	A
ATOM	2385	C	ALA	A	333	32.910	25.473	20.379	1.00	10.44	A
ATOM	2386	O	ALA	A	333	33.787	25.982	21.096	1.00	9.81	A
ATOM	2387	N	ILE	A	334	31.787	24.963	20.869	1.00	9.49	A
ATOM	2388	CA	ILE	A	334	31.536	24.919	22.305	1.00	10.34	A
ATOM	2389	CB	ILE	A	334	30.099	24.404	22.567	1.00	7.35	A
ATOM	2390	CG2	ILE	A	334	29.902	24.030	24.056	1.00	4.48	A
ATOM	2391	CG1	ILE	A	334	29.093	25.467	22.091	1.00	8.68	A
ATOM	2392	CD1	ILE	A	334	27.628	24.953	22.043	1.00	8.29	A
ATOM	2393	C	ILE	A	334	32.593	24.003	22.946	1.00	9.03	A
ATOM	2394	O	ILE	A	334	33.239	24.352	23.954	1.00	6.82	A
ATOM	2395	N	GLN	A	335	32.805	22.847	22.333	1.00	6.99	A
ATOM	2396	CA	GLN	A	335	33.800	21.903	22.831	1.00	8.99	A
ATOM	2397	CB	GLN	A	335	33.695	20.589	22.053	1.00	11.58	A
ATOM	2398	CG	GLN	A	335	32.448	19.784	22.446	1.00	21.44	A
ATOM	2399	CD	GLN	A	335	32.279	18.518	21.598	1.00	30.71	A
ATOM	2400	OE1	GLN	A	335	33.212	18.083	20.927	1.00	34.68	A
ATOM	2401	NE2	GLN	A	335	31.089	17.926	21.638	1.00	37.34	A
ATOM	2402	C	GLN	A	335	35.223	22.438	22.774	1.00	12.27	A
ATOM	2403	O	GLN	A	335	36.014	22.219	23.704	1.00	10.25	A
ATOM	2404	N	ALA	A	336	35.547	23.143	21.690	1.00	10.75	A
ATOM	2405	CA	ALA	A	336	36.868	23.726	21.514	1.00	12.71	A
ATOM	2406	CB	ALA	A	336	36.989	24.375	20.091	1.00	9.35	A
ATOM	2407	C	ALA	A	336	37.109	24.794	22.591	1.00	11.11	A
ATOM	2408	O	ALA	A	336	38.247	25.134	22.894	1.00	11.00	A
ATOM	2409	N	ASN	A	337	36.025	25.310	23.164	1.00	8.06	A
ATOM	2410	CA	ASN	A	337	36.125	26.342	24.185	1.00	9.10	A
ATOM	2411	CB	ASN	A	337	35.098	27.440	23.887	1.00	8.86	A
ATOM	2412	CG	ASN	A	337	35.621	28.457	22.874	1.00	12.21	A
ATOM	2413	OD1	ASN	A	337	36.333	29.417	23.230	1.00	12.38	A
ATOM	2414	ND2	ASN	A	337	35.301	28.237	21.605	1.00	13.95	A
ATOM	2415	C	ASN	A	337	35.979	25.816	25.622	1.00	9.52	A
ATOM	2416	O	ASN	A	337	35.647	26.565	26.534	1.00	7.92	A
ATOM	2417	N	ALA	A	338	36.242	24.523	25.806	1.00	8.29	A
ATOM	2418	CA	ALA	A	338	36.194	23.863	27.117	1.00	8.92	A
ATOM	2419	CB	ALA	A	338	37.188	24.526	28.069	1.00	10.50	A
ATOM	2420	C	ALA	A	338	34.825	23.786	27.785	1.00	8.55	A
ATOM	2421	O	ALA	A	338	34.732	23.671	29.000	1.00	10.41	A
ATOM	2422	N	PHE	A	339	33.765	23.844	27.002	1.00	7.84	A
ATOM	2423	CA	PHE	A	339	32.410	23.781	27.553	1.00	8.93	A
ATOM	2424	CB	PHE	A	339	31.624	25.034	27.120	1.00	7.76	A
ATOM	2425	CG	PHE	A	339	32.258	26.345	27.576	1.00	10.23	A
ATOM	2426	CD1	PHE	A	339	32.566	26.557	28.923	1.00	11.28	A
ATOM	2427	CD2	PHE	A	339	32.497	27.369	26.664	1.00	9.75	A

FIGURE 5 (continued)

37 / 46

ATOM	2428	CE1	PHE	A	339	33.108	27.795	29.360	1.00	11.58	A
ATOM	2429	CE2	PHE	A	339	33.033	28.613	27.077	1.00	8.17	A
ATOM	2430	CZ	PHE	A	339	33.339	28.820	28.437	1.00	8.56	A
ATOM	2431	C	PHE	A	339	31.647	22.514	27.151	1.00	9.93	A
ATOM	2432	O	PHE	A	339	32.084	21.742	26.279	1.00	9.23	A
ATOM	2433	N	VAL	A	340	30.508	22.304	27.797	1.00	8.19	A
ATOM	2434	CA	VAL	A	340	29.669	21.139	27.531	1.00	10.26	A
ATOM	2435	CB	VAL	A	340	29.169	20.468	28.851	1.00	11.72	A
ATOM	2436	CG1	VAL	A	340	28.219	19.269	28.538	1.00	8.46	A
ATOM	2437	CG2	VAL	A	340	30.346	19.998	29.679	1.00	8.91	A
ATOM	2438	C	VAL	A	340	28.439	21.577	26.742	1.00	6.33	A
ATOM	2439	O	VAL	A	340	27.675	22.433	27.186	1.00	6.81	A
ATOM	2440	N	PRO	A	341	28.255	21.021	25.547	1.00	6.85	A
ATOM	2441	CD	PRO	A	341	29.193	20.162	24.797	1.00	10.26	A
ATOM	2442	CA	PRO	A	341	27.082	21.373	24.736	1.00	9.67	A
ATOM	2443	CB	PRO	A	341	27.275	20.537	23.468	1.00	11.39	A
ATOM	2444	CG	PRO	A	341	28.752	20.386	23.363	1.00	14.97	A
ATOM	2445	C	PRO	A	341	25.807	20.931	25.497	1.00	10.96	A
ATOM	2446	O	PRO	A	341	25.851	20.024	26.342	1.00	10.96	A
ATOM	2447	N	LEU	A	342	24.673	21.558	25.211	1.00	8.13	A
ATOM	2448	CA	LEU	A	342	23.435	21.157	25.870	1.00	10.08	A
ATOM	2449	CB	LEU	A	342	22.326	22.194	25.646	1.00	12.81	A
ATOM	2450	CG	LEU	A	342	22.558	23.605	26.207	1.00	16.13	A
ATOM	2451	CD1	LEU	A	342	21.280	24.428	26.007	1.00	10.84	A
ATOM	2452	CD2	LEU	A	342	22.908	23.542	27.715	1.00	14.00	A
ATOM	2453	C	LEU	A	342	22.981	19.821	25.288	1.00	11.91	A
ATOM	2454	O	LEU	A	342	23.142	19.565	24.072	1.00	10.04	A
ATOM	2455	N	PRO	A	343	22.437	18.937	26.147	1.00	10.12	A
ATOM	2456	CD	PRO	A	343	22.407	19.074	27.618	1.00	8.23	A
ATOM	2457	CA	PRO	A	343	21.947	17.622	25.721	1.00	11.60	A
ATOM	2458	CB	PRO	A	343	21.407	17.006	27.021	1.00	11.29	A
ATOM	2459	CG	PRO	A	343	22.287	17.643	28.083	1.00	12.10	A
ATOM	2460	C	PRO	A	343	20.850	17.839	24.688	1.00	11.38	A
ATOM	2461	O	PRO	A	343	20.229	18.896	24.648	1.00	10.75	A
ATOM	2462	N	SER	A	344	20.590	16.836	23.861	1.00	9.55	A
ATOM	2463	CA	SER	A	344	19.592	16.995	22.801	1.00	8.34	A
ATOM	2464	CB	SER	A	344	19.547	15.741	21.940	1.00	15.39	A
ATOM	2465	OG	SER	A	344	19.245	14.625	22.760	1.00	23.25	A
ATOM	2466	C	SER	A	344	18.185	17.315	23.281	1.00	8.79	A
ATOM	2467	O	SER	A	344	17.474	18.051	22.615	1.00	11.06	A
ATOM	2468	N	ASN	A	345	17.751	16.744	24.410	1.00	11.97	A
ATOM	2469	CA	ASN	A	345	16.403	17.061	24.874	1.00	13.51	A
ATOM	2470	CB	ASN	A	345	15.962	16.128	26.015	1.00	11.25	A
ATOM	2471	CG	ASN	A	345	16.896	16.145	27.206	1.00	19.63	A
ATOM	2472	OD1	ASN	A	345	18.105	16.399	27.083	1.00	15.65	A
ATOM	2473	ND2	ASN	A	345	16.343	15.822	28.379	1.00	15.03	A
ATOM	2474	C	ASN	A	345	16.296	18.532	25.277	1.00	12.03	A
ATOM	2475	O	ASN	A	345	15.236	19.131	25.167	1.00	11.72	A
ATOM	2476	N	TRP	A	346	17.397	19.115	25.739	1.00	10.97	A
ATOM	2477	CA	TRP	A	346	17.397	20.533	26.097	1.00	9.55	A
ATOM	2478	CB	TRP	A	346	18.663	20.890	26.881	1.00	8.50	A
ATOM	2479	CG	TRP	A	346	18.475	20.695	28.372	1.00	9.10	A
ATOM	2480	CD2	TRP	A	346	17.927	21.660	29.285	1.00	10.08	A
ATOM	2481	CE2	TRP	A	346	17.831	21.036	30.549	1.00	12.11	A
ATOM	2482	CE3	TRP	A	346	17.502	22.994	29.149	1.00	9.60	A
ATOM	2483	CD1	TRP	A	346	18.694	19.553	29.099	1.00	9.06	A
ATOM	2484	NE1	TRP	A	346	18.304	19.752	30.411	1.00	9.93	A
ATOM	2485	CZ2	TRP	A	346	17.323	21.705	31.682	1.00	9.30	A
ATOM	2486	CZ3	TRP	A	346	17.004	23.662	30.261	1.00	10.14	A
ATOM	2487	CH2	TRP	A	346	16.917	23.012	31.522	1.00	12.99	A
ATOM	2488	C	TRP	A	346	17.298	21.390	24.824	1.00	10.69	A
ATOM	2489	O	TRP	A	346	16.509	22.333	24.769	1.00	13.16	A
ATOM	2490	N	LYS	A	347	18.087	21.074	23.804	1.00	9.34	A
ATOM	2491	CA	LYS	A	347	17.984	21.852	22.557	1.00	8.27	A
ATOM	2492	CB	LYS	A	347	18.902	21.287	21.466	1.00	12.86	A
ATOM	2493	CG	LYS	A	347	20.416	21.357	21.748	1.00	11.51	A
ATOM	2494	CD	LYS	A	347	21.221	21.071	20.440	1.00	14.73	A
ATOM	2495	CE	LYS	A	347	22.733	21.317	20.590	1.00	14.12	A
ATOM	2496	NZ	LYS	A	347	23.467	20.312	21.462	1.00	10.37	A
ATOM	2497	C	LYS	A	347	16.549	21.789	22.030	1.00	10.83	A
ATOM	2498	O	LYS	A	347	15.956	22.814	21.631	1.00	8.78	A
ATOM	2499	N	ALA	A	348	15.987	20.583	21.997	1.00	9.70	A
ATOM	2500	CA	ALA	A	348	14.627	20.418	21.472	1.00	9.41	A
ATOM	2501	CB	ALA	A	348	14.238	18.928	21.448	1.00	12.04	A
ATOM	2502	C	ALA	A	348	13.589	21.224	22.251	1.00	10.82	A
ATOM	2503	O	ALA	A	348	12.678	21.830	21.657	1.00	9.58	A

FIGURE 5 (continued)

38 / 46

ATOM	2504	N	ALA	A	349	13.735	21.261	23.569	1.00	9.39	A
ATOM	2505	CA	ALA	A	349	12.791	22.018	24.392	1.00	8.51	A
ATOM	2506	CB	ALA	A	349	13.045	21.750	25.891	1.00	8.51	A
ATOM	2507	C	ALA	A	349	12.909	23.518	24.095	1.00	10.22	A
ATOM	2508	O	ALA	A	349	11.888	24.224	24.012	1.00	8.91	A
ATOM	2509	N	VAL	A	350	14.140	24.002	23.930	1.00	12.16	A
ATOM	2510	CA	VAL	A	350	14.347	25.423	23.649	1.00	8.94	A
ATOM	2511	CB	VAL	A	350	15.863	25.794	23.629	1.00	8.30	A
ATOM	2512	CG1	VAL	A	350	16.075	27.221	23.071	1.00	8.00	A
ATOM	2513	CG2	VAL	A	350	16.439	25.729	25.075	1.00	8.81	A
ATOM	2514	C	VAL	A	350	13.709	25.763	22.305	1.00	10.89	A
ATOM	2515	O	VAL	A	350	13.046	26.787	22.177	1.00	11.46	A
ATOM	2516	N	ARG	A	351	13.890	24.895	21.313	1.00	10.91	A
ATOM	2517	CA	ARG	A	351	13.289	25.144	20.002	1.00	11.54	A
ATOM	2518	CB	ARG	A	351	13.765	24.106	18.988	1.00	10.07	A
ATOM	2519	CG	ARG	A	351	15.237	24.167	18.647	1.00	10.05	A
ATOM	2520	CD	ARG	A	351	15.527	23.433	17.312	1.00	14.16	A
ATOM	2521	NE	ARG	A	351	14.971	22.067	17.282	1.00	17.52	A
ATOM	2522	CZ	ARG	A	351	15.577	20.991	17.780	1.00	14.15	A
ATOM	2523	NH1	ARG	A	351	14.993	19.802	17.708	1.00	14.19	A
ATOM	2524	NH2	ARG	A	351	16.775	21.097	18.338	1.00	15.54	A
ATOM	2525	C	ARG	A	351	11.750	25.097	20.069	1.00	13.24	A
ATOM	2526	O	ARG	A	351	11.061	25.925	19.477	1.00	10.64	A
ATOM	2527	N	ALA	A	352	11.221	24.112	20.786	1.00	10.94	A
ATOM	2528	CA	ALA	A	352	9.772	23.942	20.890	1.00	13.45	A
ATOM	2529	CB	ALA	A	352	9.447	22.656	21.636	1.00	14.54	A
ATOM	2530	C	ALA	A	352	9.028	25.112	21.527	1.00	14.05	A
ATOM	2531	O	ALA	A	352	7.875	25.385	21.193	1.00	9.92	A
ATOM	2532	N	SER	A	353	9.669	25.802	22.454	1.00	9.51	A
ATOM	2533	CA	SER	A	353	9.024	26.932	23.094	1.00	10.39	A
ATOM	2534	CB	SER	A	353	9.503	27.088	24.548	1.00	11.56	A
ATOM	2535	OG	SER	A	353	8.802	26.220	25.436	1.00	14.83	A
ATOM	2536	C	SER	A	353	9.308	28.245	22.386	1.00	12.07	A
ATOM	2537	O	SER	A	353	8.403	29.033	22.178	1.00	12.33	A
ATOM	2538	N	TYR	A	354	10.568	28.459	22.015	1.00	10.56	A
ATOM	2539	CA	TYR	A	354	10.955	29.733	21.455	1.00	8.65	A
ATOM	2540	CB	TYR	A	354	12.240	30.188	22.159	1.00	11.42	A
ATOM	2541	CG	TYR	A	354	12.077	30.164	23.670	1.00	11.26	A
ATOM	2542	CD1	TYR	A	354	11.168	31.007	24.296	1.00	11.16	A
ATOM	2543	CE1	TYR	A	354	10.962	30.955	25.673	1.00	13.86	A
ATOM	2544	CD2	TYR	A	354	12.795	29.265	24.455	1.00	12.94	A
ATOM	2545	CE2	TYR	A	354	12.608	29.204	25.846	1.00	13.83	A
ATOM	2546	CZ	TYR	A	354	11.692	30.048	26.437	1.00	15.93	A
ATOM	2547	OH	TYR	A	354	11.496	29.985	27.784	1.00	31.84	A
ATOM	2548	C	TYR	A	354	11.069	29.882	19.951	1.00	11.12	A
ATOM	2549	O	TYR	A	354	11.137	31.011	19.456	1.00	11.00	A
ATOM	2550	N	LEU	A	355	11.097	28.778	19.218	1.00	9.87	A
ATOM	2551	CA	LEU	A	355	11.156	28.896	17.757	1.00	11.35	A
ATOM	2552	CB	LEU	A	355	12.292	28.069	17.185	1.00	12.01	A
ATOM	2553	CG	LEU	A	355	13.697	28.633	17.424	1.00	18.77	A
ATOM	2554	CD1	LEU	A	355	14.731	27.617	16.930	1.00	13.44	A
ATOM	2555	CD2	LEU	A	355	13.856	29.963	16.666	1.00	19.42	A
ATOM	2556	C	LEU	A	355	9.848	28.484	17.086	1.00	12.49	A
ATOM	2557	O	LEU	A	355	9.337	29.208	16.231	1.00	13.91	A
ATOM	2558	N	THR	A	356	9.300	27.331	17.458	1.00	13.88	A
ATOM	2559	CA	THR	A	356	8.036	26.866	16.849	1.00	16.44	A
ATOM	2560	CB	THR	A	356	7.414	25.759	17.704	1.00	19.06	A
ATOM	2561	OG1	THR	A	356	8.352	24.678	17.794	1.00	22.02	A
ATOM	2562	CG2	THR	A	356	6.108	25.265	17.077	1.00	20.44	A
ATOM	2563	C	THR	A	356	7.058	28.040	16.684	1.00	15.88	A
ATOM	2564	O	THR	A	356	6.609	28.642	17.658	1.00	14.53	A
ATOM	2565	N	ALA	A	357	6.720	28.362	15.441	1.00	16.53	A
ATOM	2566	CA	ALA	A	357	5.892	29.536	15.175	1.00	15.13	A
ATOM	2567	CB	ALA	A	357	5.654	29.669	13.662	1.00	17.87	A
ATOM	2568	C	ALA	A	357	4.569	29.630	15.918	1.00	18.27	A
ATOM	2569	O	ALA	A	357	4.141	30.714	16.295	1.00	19.17	A
ATOM	2570	N	SER	A	358	3.930	28.492	16.127	1.00	18.84	A
ATOM	2571	CA	SER	A	358	2.643	28.444	16.800	1.00	22.62	A
ATOM	2572	CB	SER	A	358	1.953	27.125	16.459	1.00	18.79	A
ATOM	2573	OG	SER	A	358	2.853	26.049	16.654	1.00	21.93	A
ATOM	2574	C	SER	A	358	2.716	28.607	18.318	1.00	22.54	A
ATOM	2575	O	SER	A	358	1.719	28.918	18.949	1.00	19.82	A
ATOM	2576	N	ASN	A	359	3.886	28.410	18.916	1.00	20.48	A
ATOM	2577	CA	ASN	A	359	3.950	28.550	20.358	1.00	16.65	A
ATOM	2578	CB	ASN	A	359	5.249	27.956	20.909	1.00	12.27	A
ATOM	2579	CG	ASN	A	359	5.180	27.718	22.387	1.00	11.80	A

FIGURE 5 (continued)

39 / 46

ATOM	2580	OD1	ASN	A	359	4.992	28.652	23.170	1.00	16.11	A
ATOM	2581	ND2	ASN	A	359	5.329	26.451	22.793	1.00	14.58	A
ATOM	2582	C	ASN	A	359	3.844	30.019	20.745	1.00	16.93	A
ATOM	2583	O	ASN	A	359	4.550	30.861	20.194	1.00	15.08	A
ATOM	2584	N	ALA	A	360	2.972	30.306	21.712	1.00	15.71	A
ATOM	2585	CA	ALA	A	360	2.759	31.664	22.208	1.00	18.67	A
ATOM	2586	CB	ALA	A	360	1.688	31.651	23.320	1.00	22.67	A
ATOM	2587	C	ALA	A	360	4.041	32.309	22.744	1.00	18.59	A
ATOM	2588	O	ALA	A	360	4.138	33.532	22.825	1.00	16.11	A
ATOM	2589	N	LEU	A	361	5.010	31.488	23.144	1.00	14.62	A
ATOM	2590	CA	LEU	A	361	6.276	32.021	23.653	1.00	11.27	A
ATOM	2591	CB	LEU	A	361	6.863	31.060	24.685	1.00	15.51	A
ATOM	2592	CG	LEU	A	361	6.087	30.788	25.971	1.00	15.37	A
ATOM	2593	CD1	LEU	A	361	6.713	29.586	26.688	1.00	15.50	A
ATOM	2594	CD2	LEU	A	361	6.086	32.030	26.849	1.00	14.07	A
ATOM	2595	C	LEU	A	361	7.334	32.219	22.545	1.00	12.87	A
ATOM	2596	O	LEU	A	361	8.430	32.716	22.818	1.00	12.41	A
ATOM	2597	N	SER	A	362	7.036	31.821	21.314	1.00	9.97	A
ATOM	2598	CA	SER	A	362	8.044	31.936	20.257	1.00	10.76	A
ATOM	2599	CB	SER	A	362	7.627	31.145	19.011	1.00	15.72	A
ATOM	2600	OG	SER	A	362	6.470	31.707	18.416	1.00	18.79	A
ATOM	2601	C	SER	A	362	8.454	33.338	19.822	1.00	12.29	A
ATOM	2602	O	SER	A	362	7.637	34.258	19.742	1.00	12.85	A
ATOM	2603	N	ILE	A	363	9.741	33.457	19.512	1.00	10.84	A
ATOM	2604	CA	ILE	A	363	10.353	34.698	19.072	1.00	14.99	A
ATOM	2605	CB	ILE	A	363	11.850	34.461	18.777	1.00	13.05	A
ATOM	2606	CG2	ILE	A	363	12.483	35.713	18.198	1.00	12.46	A
ATOM	2607	CG1	ILE	A	363	12.578	34.071	20.064	1.00	15.60	A
ATOM	2608	CD1	ILE	A	363	13.960	33.442	19.815	1.00	11.48	A
ATOM	2609	C	ILE	A	363	9.639	35.206	17.807	1.00	14.29	A
ATOM	2610	O	ILE	A	363	9.509	34.481	16.830	1.00	12.01	A
ATOM	2611	N	GLY	A	364	9.176	36.451	17.848	1.00	15.53	A
ATOM	2612	CA	GLY	A	364	8.477	37.034	16.717	1.00	14.88	A
ATOM	2613	C	GLY	A	364	7.040	36.567	16.514	1.00	19.34	A
ATOM	2614	O	GLY	A	364	6.436	36.872	15.487	1.00	19.36	A
ATOM	2615	N	ASP	A	365	6.471	35.842	17.474	1.00	15.42	A
ATOM	2616	CA	ASP	A	365	5.094	35.360	17.323	1.00	16.08	A
ATOM	2617	CB	ASP	A	365	4.625	34.691	18.613	1.00	17.24	A
ATOM	2618	CG	ASP	A	365	3.195	34.201	18.516	1.00	22.13	A
ATOM	2619	OD1	ASP	A	365	2.992	33.003	18.238	1.00	24.97	A
ATOM	2620	OD2	ASP	A	365	2.272	35.025	18.698	1.00	22.46	A
ATOM	2621	C	ASP	A	365	4.100	36.490	16.954	1.00	20.12	A
ATOM	2622	O	ASP	A	365	3.979	37.482	17.668	1.00	17.92	A
ATOM	2623	N	SER	A	366	3.379	36.317	15.848	1.00	21.25	A
ATOM	2624	CA	SER	A	366	2.419	37.319	15.360	1.00	19.32	A
ATOM	2625	CB	SER	A	366	1.704	36.787	14.108	1.00	21.13	A
ATOM	2626	OG	SER	A	366	2.640	36.400	13.125	1.00	29.92	A
ATOM	2627	C	SER	A	366	1.359	37.814	16.342	1.00	15.84	A
ATOM	2628	O	SER	A	366	1.155	39.010	16.461	1.00	22.39	A
ATOM	2629	N	ALA	A	367	0.655	36.920	17.024	1.00	18.40	A
ATOM	2630	CA	ALA	A	367	-0.384	37.363	17.965	1.00	22.33	A
ATOM	2631	CB	ALA	A	367	-1.220	36.175	18.431	1.00	19.13	A
ATOM	2632	C	ALA	A	367	0.182	38.093	19.187	1.00	25.24	A
ATOM	2633	O	ALA	A	367	-0.402	39.066	19.682	1.00	26.45	A
ATOM	2634	N	VAL	A	368	1.311	37.612	19.692	1.00	24.39	A
ATOM	2635	CA	VAL	A	368	1.903	38.229	20.864	1.00	21.43	A
ATOM	2636	CB	VAL	A	368	2.729	37.182	21.657	1.00	23.84	A
ATOM	2637	CG1	VAL	A	368	3.447	37.838	22.850	1.00	19.42	A
ATOM	2638	CG2	VAL	A	368	1.810	36.094	22.148	1.00	25.28	A
ATOM	2639	C	VAL	A	368	2.770	39.447	20.558	1.00	19.50	A
ATOM	2640	O	VAL	A	368	2.713	40.440	21.277	1.00	22.77	A
ATOM	2641	N	CYS	A	369	3.557	39.396	19.491	1.00	17.47	A
ATOM	2642	CA	CYS	A	369	4.448	40.505	19.195	1.00	20.32	A
ATOM	2643	C	CYS	A	369	3.919	41.648	18.322	1.00	23.64	A
ATOM	2644	O	CYS	A	369	4.617	42.639	18.120	1.00	26.98	A
ATOM	2645	CB	CYS	A	369	5.746	39.977	18.581	1.00	22.42	A
ATOM	2646	SG	CYS	A	369	6.819	38.961	19.671	1.00	19.53	A
ATOM	2647	N	GLY	A	370	2.698	41.521	17.812	1.00	25.38	A
ATOM	2648	CA	GLY	A	370	2.154	42.575	16.966	1.00	27.80	A
ATOM	2649	C	GLY	A	370	2.190	43.938	17.627	1.00	21.46	A
ATOM	2650	O	GLY	A	370	1.631	44.112	18.705	1.00	25.76	A
ATOM	2651	N	GLY	A	371	2.872	44.885	16.988	1.00	20.44	A
ATOM	2652	CA	GLY	A	371	2.970	46.237	17.516	1.00	23.12	A
ATOM	2653	C	GLY	A	371	3.913	46.463	18.695	1.00	26.63	A
ATOM	2654	O	GLY	A	371	3.946	47.561	19.263	1.00	23.97	A
ATOM	2655	N	LYS	A	372	4.689	45.443	19.057	1.00	23.24	A

FIGURE 5 (continued)

40 / 46

ATOM	2656	CA	LYS	A	372	5.612	45.537	20.197	1.00	21.66	A
ATOM	2657	CB	LYS	A	372	5.141	44.605	21.296	1.00	19.20	A
ATOM	2658	CG	LYS	A	372	3.715	44.856	21.675	1.00	25.31	A
ATOM	2659	CD	LYS	A	372	3.278	43.936	22.769	1.00	24.34	A
ATOM	2660	CE	LYS	A	372	1.884	44.315	23.208	1.00	29.63	A
ATOM	2661	NZ	LYS	A	372	1.426	43.423	24.285	1.00	25.95	A
ATOM	2662	C	LYS	A	372	7.037	45.167	19.855	1.00	18.74	A
ATOM	2663	O	LYS	A	372	7.337	44.799	18.721	1.00	17.43	A
ATOM	2664	N	GLY	A	373	7.917	45.247	20.852	1.00	15.44	A
ATOM	2665	CA	GLY	A	373	9.297	44.876	20.616	1.00	12.87	A
ATOM	2666	C	GLY	A	373	10.366	45.876	21.015	1.00	17.42	A
ATOM	2667	O	GLY	A	373	10.168	47.106	20.965	1.00	13.70	A
ATOM	2668	N	ARG	A	374	11.517	45.342	21.419	1.00	14.49	A
ATOM	2669	CA	ARG	A	374	12.639	46.187	21.792	1.00	13.29	A
ATOM	2670	CB	ARG	A	374	13.786	45.339	22.333	1.00	15.72	A
ATOM	2671	CG	ARG	A	374	13.456	44.710	23.692	1.00	18.10	A
ATOM	2672	CD	ARG	A	374	14.668	44.080	24.332	1.00	20.11	A
ATOM	2673	NE	ARG	A	374	15.729	45.034	24.665	1.00	13.47	A
ATOM	2674	CZ	ARG	A	374	16.143	45.296	25.899	1.00	13.50	A
ATOM	2675	NH1	ARG	A	374	15.564	44.694	26.928	1.00	11.14	A
ATOM	2676	NH2	ARG	A	374	17.206	46.082	26.100	1.00	9.65	A
ATOM	2677	C	ARG	A	374	13.097	46.989	20.563	1.00	14.09	A
ATOM	2678	O	ARG	A	374	13.008	46.517	19.411	1.00	13.90	A
ATOM	2679	N	PRO	A	375	13.575	48.225	20.797	1.00	13.52	A
ATOM	2680	CD	PRO	A	375	13.680	48.834	22.133	1.00	12.37	A
ATOM	2681	CA	PRO	A	375	14.051	49.137	19.753	1.00	15.51	A
ATOM	2682	CB	PRO	A	375	14.304	50.445	20.516	1.00	18.56	A
ATOM	2683	CG	PRO	A	375	14.669	49.958	21.903	1.00	16.56	A
ATOM	2684	C	PRO	A	375	15.282	48.622	19.017	1.00	16.94	A
ATOM	2685	O	PRO	A	375	16.130	47.953	19.605	1.00	16.29	A
ATOM	2686	N	GLU	A	376	15.384	48.956	17.733	1.00	14.83	A
ATOM	2687	CA	GLU	A	376	16.501	48.480	16.928	1.00	14.54	A
ATOM	2688	CB	GLU	A	376	16.191	48.638	15.429	1.00	20.94	A
ATOM	2689	CG	GLU	A	376	15.989	50.054	14.930	1.00	25.93	A
ATOM	2690	CD	GLU	A	376	15.840	50.093	13.408	1.00	28.12	A
ATOM	2691	OE1	GLU	A	376	16.852	50.265	12.693	1.00	27.73	A
ATOM	2692	OE2	GLU	A	376	14.706	49.921	12.926	1.00	22.85	A
ATOM	2693	C	GLU	A	376	17.818	49.144	17.258	1.00	15.46	A
ATOM	2694	O	GLU	A	376	17.779	50.308	17.715	1.00	20.34	A
ATOM	2695	OXT	GLU	A	376	18.870	48.501	17.040	1.00	17.16	A
ATOM	2696	OH2	WAT	S1500		35.620	33.372	34.950	1.00	7.74	S
ATOM	2697	OH2	WAT	S1501		26.719	26.585	54.115	1.00	13.35	S
ATOM	2698	OH2	WAT	S1502		32.910	38.720	42.612	1.00	11.02	S
ATOM	2699	OH2	WAT	S1503		25.842	40.990	19.393	1.00	10.30	S
ATOM	2700	OH2	WAT	S1504		47.855	24.508	32.439	1.00	11.64	S
ATOM	2701	OH2	WAT	S1505		37.575	38.877	30.460	1.00	13.25	S
ATOM	2702	OH2	WAT	S1506		43.970	19.166	36.360	1.00	11.89	S
ATOM	2703	OH2	WAT	S1507		51.431	26.280	38.870	1.00	11.08	S
ATOM	2704	OH2	WAT	S1508		21.180	34.238	33.496	1.00	10.94	S
ATOM	2705	OH2	WAT	S1509		34.016	23.145	55.150	1.00	7.21	S
ATOM	2706	OH2	WAT	S1510		34.137	35.767	50.996	1.00	14.32	S
ATOM	2707	OH2	WAT	S1511		29.833	31.064	61.815	1.00	12.62	S
ATOM	2708	OH2	WAT	S1512		36.421	34.348	51.750	1.00	8.81	S
ATOM	2709	OH2	WAT	S1513		24.593	22.841	22.601	1.00	14.49	S
ATOM	2710	OH2	WAT	S1514		33.875	20.919	53.336	1.00	15.73	S
ATOM	2711	OH2	WAT	S1515		55.590	18.894	44.228	1.00	20.22	S
ATOM	2712	OH2	WAT	S1516		25.163	24.507	19.298	1.00	7.32	S
ATOM	2713	OH2	WAT	S1517		29.287	27.565	53.584	1.00	10.43	S
ATOM	2714	OH2	WAT	S1518		27.630	35.157	54.573	1.00	11.84	S
ATOM	2715	OH2	WAT	S1519		34.308	40.814	45.314	1.00	9.91	S
ATOM	2716	OH2	WAT	S1520		24.097	26.340	47.444	1.00	12.35	S
ATOM	2717	OH2	WAT	S1521		26.289	17.353	26.191	1.00	14.15	S
ATOM	2718	OH2	WAT	S1522		31.025	26.248	57.309	1.00	9.97	S
ATOM	2719	OH2	WAT	S1523		16.012	33.323	36.822	1.00	10.61	S
ATOM	2720	OH2	WAT	S1524		35.079	31.981	26.882	1.00	7.27	S
ATOM	2721	OH2	WAT	S1525		48.948	16.302	35.666	1.00	22.32	S
ATOM	2722	OH2	WAT	S1526		23.036	32.247	50.228	1.00	12.80	S
ATOM	2723	OH2	WAT	S1527		41.445	42.204	48.819	1.00	16.71	S
ATOM	2724	OH2	WAT	S1528		30.777	34.835	16.827	1.00	12.96	S
ATOM	2725	OH2	WAT	S1529		9.482	33.895	27.983	1.00	10.22	S
ATOM	2726	OH2	WAT	S1530		10.107	31.646	29.601	1.00	12.12	S
ATOM	2727	OH2	WAT	S1531		37.836	31.446	58.127	1.00	18.63	S
ATOM	2728	OH2	WAT	S1532		23.419	29.528	35.937	1.00	10.10	S
ATOM	2729	OH2	WAT	S1533		36.234	16.727	51.505	1.00	9.28	S
ATOM	2730	OH2	WAT	S1534		5.728	38.503	24.985	1.00	13.33	S
ATOM	2731	OH2	WAT	S1535		29.914	14.295	35.432	1.00	16.41	S

FIGURE 5 (continued)

41 / 46

ATOM	2732	OH2	WAT	S1536	31.310	38.281	18.695	1.00	9.93	S
ATOM	2733	OH2	WAT	S1537	44.863	16.606	36.022	1.00	15.09	S
ATOM	2734	OH2	WAT	S1538	40.186	22.869	38.700	1.00	9.90	S
ATOM	2735	OH2	WAT	S1539	37.549	20.501	28.090	1.00	13.36	S
ATOM	2736	OH2	WAT	S1540	12.913	31.829	29.436	1.00	9.36	S
ATOM	2737	OH2	WAT	S1541	30.589	15.671	37.530	1.00	12.47	S
ATOM	2738	OH2	WAT	S1542	23.885	35.406	43.402	1.00	18.37	S
ATOM	2739	OH2	WAT	S1543	8.663	34.010	25.289	1.00	13.37	S
ATOM	2740	OH2	WAT	S1544	13.484	46.444	33.757	1.00	12.24	S
ATOM	2741	OH2	WAT	S1545	27.923	19.477	57.944	1.00	11.68	S
ATOM	2742	OH2	WAT	S1546	17.540	33.345	7.715	1.00	19.22	S
ATOM	2743	OH2	WAT	S1547	51.552	13.602	41.885	1.00	25.84	S
ATOM	2744	OH2	WAT	S1548	27.270	26.074	40.675	1.00	10.51	S
ATOM	2745	OH2	WAT	S1549	27.760	43.771	20.816	1.00	13.46	S
ATOM	2746	OH2	WAT	S1550	37.046	17.292	27.914	1.00	14.34	S
ATOM	2747	OH2	WAT	S1551	37.573	33.819	20.741	1.00	23.07	S
ATOM	2748	OH2	WAT	S1552	40.930	14.067	35.565	1.00	17.08	S
ATOM	2749	OH2	WAT	S1553	4.472	29.061	32.567	1.00	18.41	S
ATOM	2750	OH2	WAT	S1554	26.302	32.912	28.375	1.00	10.00	S
ATOM	2751	OH2	WAT	S1555	14.165	45.737	16.934	1.00	13.06	S
ATOM	2752	OH2	WAT	S1556	29.555	43.029	36.030	1.00	7.32	S
ATOM	2753	OH2	WAT	S1557	36.451	34.819	37.298	1.00	11.33	S
ATOM	2754	OH2	WAT	S1558	31.931	17.255	49.603	1.00	39.16	S
ATOM	2755	OH2	WAT	S1559	23.622	26.926	37.001	1.00	11.87	S
ATOM	2756	OH2	WAT	S1560	31.327	13.311	33.059	1.00	12.47	S
ATOM	2757	OH2	WAT	S1561	44.899	41.787	36.741	1.00	23.25	S
ATOM	2758	OH2	WAT	S1562	44.879	35.365	50.334	1.00	9.60	S
ATOM	2759	OH2	WAT	S1563	20.827	50.011	18.100	1.00	15.06	S
ATOM	2760	OH2	WAT	S1564	24.374	31.041	38.304	1.00	12.38	S
ATOM	2761	OH2	WAT	S1565	11.411	42.003	26.114	1.00	14.55	S
ATOM	2762	OH2	WAT	S1566	21.341	35.751	40.722	1.00	12.16	S
ATOM	2763	OH2	WAT	S1567	10.175	31.393	39.888	1.00	37.76	S
ATOM	2764	OH2	WAT	S1568	47.181	26.945	33.704	1.00	12.30	S
ATOM	2765	OH2	WAT	S1569	42.028	43.488	36.919	1.00	25.46	S
ATOM	2766	OH2	WAT	S1570	31.053	24.724	15.706	1.00	12.46	S
ATOM	2767	OH2	WAT	S1571	10.314	39.156	33.480	1.00	10.32	S
ATOM	2768	OH2	WAT	S1572	51.433	20.485	50.130	1.00	15.09	S
ATOM	2769	OH2	WAT	S1573	43.925	30.656	51.790	1.00	17.28	S
ATOM	2770	OH2	WAT	S1574	23.091	53.758	28.375	1.00	12.50	S
ATOM	2771	OH2	WAT	S1575	34.977	41.183	53.019	1.00	15.31	S
ATOM	2772	OH2	WAT	S1576	29.766	26.781	12.309	1.00	18.82	S
ATOM	2773	OH2	WAT	S1577	9.190	36.561	30.593	1.00	11.25	S
ATOM	2774	OH2	WAT	S1578	36.599	15.728	48.666	1.00	21.18	S
ATOM	2775	OH2	WAT	S1579	37.724	34.865	54.143	1.00	11.62	S
ATOM	2776	OH2	WAT	S1580	21.457	35.713	12.303	1.00	13.24	S
ATOM	2777	OH2	WAT	S1581	27.734	31.073	59.797	1.00	14.78	S
ATOM	2778	OH2	WAT	S1582	51.536	35.554	40.163	1.00	14.52	S
ATOM	2779	OH2	WAT	S1583	29.933	42.651	53.057	1.00	14.55	S
ATOM	2780	OH2	WAT	S1584	9.469	23.677	25.125	1.00	12.14	S
ATOM	2781	OH2	WAT	S1585	20.704	29.372	11.334	1.00	17.80	S
ATOM	2782	OH2	WAT	S1586	56.481	22.975	38.435	1.00	29.16	S
ATOM	2783	OH2	WAT	S1587	9.572	40.421	17.037	1.00	14.99	S
ATOM	2784	OH2	WAT	S1588	20.542	42.224	40.862	1.00	13.90	S
ATOM	2785	OH2	WAT	S1589	9.567	37.848	39.841	1.00	15.10	S
ATOM	2786	OH2	WAT	S1590	6.391	48.835	28.636	1.00	19.52	S
ATOM	2787	OH2	WAT	S1591	41.492	20.894	55.469	1.00	16.40	S
ATOM	2788	OH2	WAT	S1592	22.505	28.556	52.952	1.00	24.23	S
ATOM	2789	OH2	WAT	S1593	27.720	46.441	20.204	1.00	15.40	S
ATOM	2790	OH2	WAT	S1594	37.216	41.499	30.864	1.00	19.68	S
ATOM	2791	OH2	WAT	S1595	30.199	27.159	15.034	1.00	11.19	S
ATOM	2792	OH2	WAT	S1596	25.139	30.964	53.858	1.00	21.47	S
ATOM	2793	OH2	WAT	S1597	35.730	20.698	18.767	1.00	15.15	S
ATOM	2794	OH2	WAT	S1598	44.994	20.666	23.797	1.00	17.67	S
ATOM	2795	OH2	WAT	S1599	28.802	58.069	26.514	1.00	17.28	S
ATOM	2796	OH2	WAT	S1600	16.767	47.104	22.319	1.00	11.98	S
ATOM	2797	OH2	WAT	S1601	30.159	33.756	60.797	1.00	9.19	S
ATOM	2798	OH2	WAT	S1602	48.106	27.997	36.005	1.00	14.93	S
ATOM	2799	OH2	WAT	S1603	40.650	24.407	21.552	1.00	17.12	S
ATOM	2800	OH2	WAT	S1604	22.968	17.449	18.008	1.00	17.85	S
ATOM	2801	OH2	WAT	S1605	16.621	15.788	18.605	1.00	25.68	S
ATOM	2802	OH2	WAT	S1606	7.206	32.992	16.005	1.00	14.53	S
ATOM	2803	OH2	WAT	S1607	57.149	24.564	47.629	1.00	18.35	S
ATOM	2804	OH2	WAT	S1608	24.205	26.840	10.350	1.00	23.21	S
ATOM	2805	OH2	WAT	S1609	33.745	22.604	31.364	1.00	14.24	S
ATOM	2806	OH2	WAT	S1610	21.687	28.608	49.750	1.00	41.13	S
ATOM	2807	OH2	WAT	S1611	25.572	18.289	18.085	1.00	18.47	S

FIGURE 5 (continued)

42 / 46

ATOM	2808	OH2	WAT	S1612	29.378	22.049	15.378	1.00	18.53	S
ATOM	2809	OH2	WAT	S1613	47.580	17.180	46.156	1.00	18.00	S
ATOM	2810	OH2	WAT	S1614	23.216	43.309	37.644	1.00	13.17	S
ATOM	2811	OH2	WAT	S1615	22.669	24.274	48.564	1.00	24.15	S
ATOM	2812	OH2	WAT	S1616	0.336	31.433	18.582	1.00	27.87	S
ATOM	2813	OH2	WAT	S1617	45.294	33.053	51.773	1.00	13.88	S
ATOM	2814	OH2	WAT	S1618	44.363	26.868	22.624	1.00	23.01	S
ATOM	2815	OH2	WAT	S1619	24.023	16.291	14.532	1.00	14.28	S
ATOM	2816	OH2	WAT	S1620	25.803	16.259	28.626	1.00	18.77	S
ATOM	2817	OH2	WAT	S1621	10.423	51.944	32.078	1.00	36.29	S
ATOM	2818	OH2	WAT	S1622	26.115	58.809	27.014	1.00	15.64	S
ATOM	2819	OH2	WAT	S1623	1.344	28.356	22.672	1.00	26.37	S
ATOM	2820	OH2	WAT	S1624	26.639	58.198	21.115	1.00	25.02	S
ATOM	2821	OH2	WAT	S1625	26.622	32.997	55.284	1.00	16.24	S
ATOM	2822	OH2	WAT	S1626	15.027	52.473	26.183	1.00	21.76	S
ATOM	2823	OH2	WAT	S1627	57.187	25.783	44.900	1.00	20.20	S
ATOM	2824	OH2	WAT	S1628	44.922	43.322	47.514	1.00	18.96	S
ATOM	2825	OH2	WAT	S1629	32.001	38.779	53.199	1.00	17.42	S
ATOM	2826	OH2	WAT	S1630	30.741	52.390	22.108	1.00	18.11	S
ATOM	2827	OH2	WAT	S1631	14.999	39.258	44.162	1.00	19.15	S
ATOM	2828	OH2	WAT	S1632	44.210	20.606	55.552	1.00	17.79	S
ATOM	2829	OH2	WAT	S1633	21.471	43.377	12.416	1.00	19.05	S
ATOM	2830	OH2	WAT	S1634	13.869	15.823	31.777	1.00	25.21	S
ATOM	2831	OH2	WAT	S1635	52.620	30.612	55.173	1.00	30.08	S
ATOM	2832	OH2	WAT	S1636	26.556	19.486	52.050	1.00	29.07	S
ATOM	2833	OH2	WAT	S1637	21.965	25.980	45.841	1.00	19.07	S
ATOM	2834	OH2	WAT	S1638	51.617	33.897	42.473	1.00	9.81	S
ATOM	2835	OH2	WAT	S1639	11.552	20.655	19.351	1.00	16.68	S
ATOM	2836	OH2	WAT	S1640	30.899	45.201	19.222	1.00	26.19	S
ATOM	2837	OH2	WAT	S1641	31.709	48.342	31.000	1.00	18.10	S
ATOM	2838	OH2	WAT	S1642	23.676	25.327	22.818	1.00	14.28	S
ATOM	2839	OH2	WAT	S1643	25.577	17.219	46.479	1.00	20.91	S
ATOM	2840	OH2	WAT	S1644	18.005	18.283	19.152	1.00	24.14	S
ATOM	2841	OH2	WAT	S1645	52.881	16.705	50.095	1.00	20.16	S
ATOM	2842	OH2	WAT	S1646	5.848	42.562	37.856	1.00	19.01	S
ATOM	2843	OH2	WAT	S1647	43.582	14.659	34.565	1.00	28.17	S
ATOM	2844	OH2	WAT	S1648	22.374	17.743	20.886	1.00	18.81	S
ATOM	2845	OH2	WAT	S1649	8.712	48.989	27.030	1.00	23.87	S
ATOM	2846	OH2	WAT	S1650	2.521	47.157	34.228	1.00	30.10	S
ATOM	2847	OH2	WAT	S1651	44.220	43.064	40.109	1.00	29.97	S
ATOM	2848	OH2	WAT	S1652	27.919	24.353	12.179	1.00	16.62	S
ATOM	2849	OH2	WAT	S1653	3.523	42.077	26.249	1.00	22.83	S
ATOM	2850	OH2	WAT	S1654	20.380	44.291	37.672	1.00	17.30	S
ATOM	2851	OH2	WAT	S1655	57.034	28.423	45.056	1.00	27.44	S
ATOM	2852	OH2	WAT	S1656	49.668	24.467	30.455	1.00	22.73	S
ATOM	2853	OH2	WAT	S1657	51.259	13.409	45.586	1.00	34.23	S
ATOM	2854	OH2	WAT	S1658	9.456	23.136	36.163	1.00	24.71	S
ATOM	2855	OH2	WAT	S1659	52.331	23.665	57.905	1.00	18.92	S
ATOM	2856	OH2	WAT	S1660	43.381	40.535	56.268	1.00	30.03	S
ATOM	2857	OH2	WAT	S1661	13.806	46.776	43.159	1.00	30.72	S
ATOM	2858	OH2	WAT	S1662	53.981	30.491	48.223	1.00	13.32	S
ATOM	2859	OH2	WAT	S1663	41.765	26.570	28.744	1.00	27.76	S
ATOM	2860	OH2	WAT	S1664	40.737	17.318	53.732	1.00	24.67	S
ATOM	2861	OH2	WAT	S1665	13.225	44.990	8.674	1.00	28.84	S
ATOM	2862	OH2	WAT	S1666	49.013	41.254	39.651	1.00	28.00	S
ATOM	2863	OH2	WAT	S1667	44.805	37.426	30.933	1.00	16.56	S
ATOM	2864	OH2	WAT	S1668	43.625	18.020	54.500	1.00	24.62	S
ATOM	2865	OH2	WAT	S1669	14.317	25.699	46.118	1.00	34.64	S
ATOM	2866	OH2	WAT	S1670	3.256	42.913	32.109	1.00	29.06	S
ATOM	2867	OH2	WAT	S1671	10.555	49.763	20.725	1.00	28.19	S
ATOM	2868	OH2	WAT	S1672	10.096	51.223	27.611	1.00	23.49	S
ATOM	2869	OH2	WAT	S1673	14.363	23.946	36.209	1.00	40.49	S
ATOM	2870	OH2	WAT	S1674	25.126	59.432	22.831	1.00	22.37	S
ATOM	2871	OH2	WAT	S1675	36.093	4.004	46.425	1.00	41.05	S
ATOM	2872	OH2	WAT	S1676	58.346	33.177	43.906	1.00	32.25	S
ATOM	2873	OH2	WAT	S1677	48.932	35.192	51.801	1.00	26.68	S
ATOM	2874	OH2	WAT	S1678	58.902	19.301	43.107	1.00	25.48	S
ATOM	2875	OH2	WAT	S1679	44.340	42.085	50.822	1.00	28.00	S
ATOM	2876	OH2	WAT	S1680	50.480	38.266	34.016	1.00	31.92	S
ATOM	2877	OH2	WAT	S1681	32.259	20.178	55.706	1.00	22.68	S
ATOM	2878	OH2	WAT	S1682	5.907	48.823	21.778	1.00	41.37	S
ATOM	2879	OH2	WAT	S1683	50.286	29.738	36.205	1.00	41.24	S
ATOM	2880	OH2	WAT	S1684	48.359	24.392	27.682	1.00	21.59	S
ATOM	2881	OH2	WAT	S1685	28.819	16.491	25.944	1.00	22.91	S
ATOM	2882	OH2	WAT	S1686	27.814	39.366	53.598	1.00	22.13	S
ATOM	2883	OH2	WAT	S1687	23.282	56.182	29.647	1.00	21.73	S

FIGURE 5 (continued)

43 / 46

ATOM	2884	OII2	WAT	S1688	11.176	51.488	23.245	1.00	39.40	S
ATOM	2885	OII2	WAT	S1689	19.333	13.893	25.470	1.00	16.29	S
ATOM	2886	OH2	WAT	S1690	15.528	35.966	43.442	1.00	24.55	S
ATOM	2887	OH2	WAT	S1691	28.485	18.098	54.189	1.00	38.82	S
ATOM	2888	OH2	WAT	S1692	49.461	42.346	42.415	1.00	29.71	S
ATOM	2889	OH2	WAT	S1693	6.986	51.318	31.491	1.00	38.19	S
ATOM	2890	OH2	WAT	S1694	45.805	30.330	30.352	1.00	31.74	S
ATOM	2891	OH2	WAT	S1695	12.688	17.949	24.810	1.00	24.29	S
ATOM	2892	OH2	WAT	S1696	10.481	44.192	41.405	1.00	30.36	S
ATOM	2893	OII2	WAT	S1697	36.497	25.163	61.042	1.00	22.75	S
ATOM	2894	OH2	WAT	S1698	38.997	8.895	40.582	1.00	35.83	S
ATOM	2895	OH2	WAT	S1699	34.429	41.271	24.603	1.00	25.66	S
ATOM	2896	OH2	WAT	S1700	9.264	39.356	31.031	1.00	12.79	S
ATOM	2897	OH2	WAT	S1701	10.070	23.977	42.971	1.00	38.68	S
ATOM	2898	OH2	WAT	S1702	18.383	29.372	9.706	1.00	36.59	S
ATOM	2899	OH2	WAT	S1703	49.044	14.511	44.663	1.00	29.13	S
ATOM	2900	OH2	WAT	S1704	24.559	26.271	39.612	1.00	9.57	S
ATOM	2901	OH2	WAT	S1705	20.114	45.757	12.779	1.00	24.18	S
ATOM	2902	OH2	WAT	S1706	40.248	22.113	20.074	1.00	29.44	S
ATOM	2903	OH2	WAT	S1707	18.194	41.869	42.229	1.00	17.46	S
ATOM	2904	OH2	WAT	S1708	37.847	20.546	20.498	1.00	18.73	S
ATOM	2905	OH2	WAT	S1709	16.821	29.280	41.001	1.00	24.06	S
ATOM	2906	OH2	WAT	S1710	27.294	42.193	52.815	1.00	19.46	S
ATOM	2907	OH2	WAT	S1711	40.821	42.347	51.556	1.00	22.66	S
ATOM	2908	OII2	WAT	S1712	26.156	40.106	48.095	1.00	24.85	S
ATOM	2909	OII2	WAT	S1713	20.103	24.718	47.608	1.00	30.63	S
ATOM	2910	OH2	WAT	S1714	24.148	33.741	56.397	1.00	19.34	S
ATOM	2911	OII2	WAT	S1715	18.973	45.993	36.285	1.00	18.68	S
ATOM	2912	OH2	WAT	S1716	14.529	44.714	35.623	1.00	11.98	S
ATOM	2913	OII2	WAT	S1717	38.781	35.753	22.003	1.00	28.14	S
ATOM	2914	OH2	WAT	S1718	9.031	37.190	34.220	1.00	30.97	S
ATOM	2915	OH2	WAT	S1719	35.994	16.311	25.745	1.00	28.93	S
ATOM	2916	OH2	WAT	S1720	13.544	49.140	34.673	1.00	19.62	S
ATOM	2917	OH2	WAT	S1721	22.265	37.832	42.637	1.00	21.65	S
ATOM	2918	OH2	WAT	S1722	9.246	42.739	13.991	1.00	23.76	S
ATOM	2919	OH2	WAT	S1723	46.901	14.013	46.528	1.00	24.08	S
ATOM	2920	OH2	WAT	S1724	27.124	17.124	56.373	1.00	20.76	S
ATOM	2921	OH2	WAT	S1725	5.808	39.927	37.880	1.00	30.10	S
ATOM	2922	OH2	WAT	S1726	42.361	20.811	20.431	1.00	24.61	S
ATOM	2923	OII2	WAT	S1727	26.665	17.537	21.374	1.00	22.27	S
ATOM	2924	OH2	WAT	S1728	57.473	29.684	48.797	1.00	33.94	S
ATOM	2925	OII2	WAT	S1729	0.205	29.580	11.300	1.00	28.38	S
ATOM	2926	OH2	WAT	S1730	28.982	12.144	36.663	1.00	22.16	S
ATOM	2927	OH2	WAT	S1731	-2.247	31.885	18.386	1.00	37.56	S
ATOM	2928	OH2	WAT	S1732	19.593	14.821	28.910	1.00	29.82	S
ATOM	2929	OH2	WAT	S1733	1.174	27.052	34.363	1.00	22.10	S
ATOM	2930	OH2	WAT	S1734	35.909	11.924	47.248	1.00	27.93	S
ATOM	2931	OH2	WAT	S1735	41.887	40.436	52.838	1.00	28.22	S
ATOM	2932	OH2	WAT	S1736	26.213	19.454	10.997	1.00	22.64	S
ATOM	2933	OII2	WAT	S1737	34.114	42.884	34.175	1.00	28.42	S
ATOM	2934	OH2	WAT	S1738	22.945	32.302	53.065	1.00	25.85	S
ATOM	2935	OII2	WAT	S1739	39.089	15.172	28.466	1.00	31.20	S
ATOM	2936	OH2	WAT	S1740	47.610	43.601	46.621	1.00	36.15	S
ATOM	2937	OH2	WAT	S1741	16.327	45.853	37.179	1.00	17.39	S
ATOM	2938	OII2	WAT	S1742	55.363	25.260	59.367	1.00	29.21	S
ATOM	2939	OII2	WAT	S1743	30.641	36.731	14.630	1.00	26.83	S
ATOM	2940	OH2	WAT	S1744	10.864	46.250	10.531	1.00	23.96	S
ATOM	2941	OII2	WAT	S1745	33.170	48.399	28.312	1.00	27.45	S
ATOM	2942	OH2	WAT	S1746	32.054	14.892	42.067	1.00	24.32	S
ATOM	2943	OH2	WAT	S1747	42.724	28.782	21.018	1.00	34.32	S
ATOM	2944	OH2	WAT	S1748	51.123	15.697	52.194	1.00	27.97	S
ATOM	2945	OII2	WAT	S1749	42.354	43.166	56.140	1.00	29.49	S
ATOM	2946	OH2	WAT	S1750	28.037	37.891	13.736	1.00	33.67	S
ATOM	2947	OII2	WAT	S1751	51.086	26.646	30.768	1.00	30.84	S
ATOM	2948	OH2	WAT	S1752	10.931	38.592	10.467	1.00	25.71	S
ATOM	2949	OII2	WAT	S1753	25.655	29.886	60.929	1.00	19.64	S
ATOM	2950	OH2	WAT	S1754	17.145	13.376	23.383	1.00	34.23	S
ATOM	2951	OII2	WAT	S1755	44.748	12.372	45.391	1.00	18.99	S
ATOM	2952	OII2	WAT	S1756	24.658	10.868	33.101	1.00	39.56	S
ATOM	2953	OII2	WAT	S1757	10.322	35.265	39.792	1.00	31.55	S
ATOM	2954	OH2	WAT	S1758	57.341	22.537	45.377	1.00	16.36	S
ATOM	2955	OH2	WAT	S1759	9.420	34.820	36.963	1.00	32.92	S
ATOM	2956	OH2	WAT	S1760	32.502	28.596	14.854	1.00	21.37	S
ATOM	2957	OH2	WAT	S1761	39.205	22.929	17.441	1.00	35.60	S
ATOM	2958	OH2	WAT	S1762	20.840	52.812	17.278	1.00	31.30	S
ATOM	2959	OH2	WAT	S1763	34.711	11.735	35.138	1.00	32.11	S

FIGURE 5 (continued)

44 / 46

ATOM	2960	OH2	WAT	S1764	51.666	34.131	47.365	1.00	35.34	S
ATOM	2961	OH2	WAT	S1765	-2.014	36.180	15.830	1.00	28.16	S
ATOM	2962	OH2	WAT	S1766	15.482	48.721	37.060	1.00	29.26	S
ATOM	2963	OH2	WAT	S1767	40.630	14.716	31.062	1.00	40.40	S
ATOM	2964	OH2	WAT	S1768	23.698	61.256	21.533	1.00	16.86	S
ATOM	2965	OH2	WAT	S1769	24.781	28.532	54.977	1.00	16.20	S
ATOM	2966	OH2	WAT	S1770	26.852	25.257	10.061	1.00	30.41	S
ATOM	2967	OH2	WAT	S1771	43.726	10.405	46.878	1.00	29.13	S
ATOM	2968	OH2	WAT	S1772	25.837	37.362	54.027	1.00	21.97	S
ATOM	2969	OH2	WAT	S1773	33.373	46.686	32.566	1.00	26.20	S
ATOM	2970	OH2	WAT	S1774	27.264	20.817	13.545	1.00	22.02	S
ATOM	2971	OH2	WAT	S1775	47.925	30.806	31.477	1.00	33.49	S
ATOM	2972	OH2	WAT	S1776	8.238	38.202	37.592	1.00	26.28	S
ATOM	2973	OH2	WAT	S1777	21.090	51.641	25.222	1.00	18.54	S
ATOM	2974	OH2	WAT	S1778	6.267	38.069	32.873	1.00	22.17	S
ATOM	2975	OH2	WAT	S1779	23.234	49.347	16.745	1.00	24.08	S
ATOM	2976	OH2	WAT	S1780	22.134	39.856	40.656	1.00	21.00	S
ATOM	2977	OH2	WAT	S1781	20.856	35.405	9.637	1.00	23.13	S
ATOM	2978	OH2	WAT	S1782	21.475	53.999	26.047	1.00	27.01	S
ATOM	2979	OH2	WAT	S1783	34.915	27.212	15.190	1.00	31.71	S
ATOM	2980	OH2	WAT	S1784	45.211	12.993	42.137	1.00	21.38	S
ATOM	2981	OH2	WAT	S1785	38.126	34.805	40.034	1.00	17.57	S
ATOM	2982	OH2	WAT	S1786	30.962	49.798	21.332	1.00	32.31	S
ATOM	2983	OH2	WAT	S1787	33.222	19.319	25.705	1.00	29.22	S
ATOM	2984	OH2	WAT	S1788	40.144	19.662	28.253	1.00	33.93	S
ATOM	2985	OH2	WAT	S1789	6.555	28.590	37.281	1.00	28.90	S
ATOM	2986	OH2	WAT	S1790	43.426	43.935	45.155	1.00	34.35	S
ATOM	2987	OH2	WAT	S1791	3.263	33.201	14.705	1.00	33.11	S
ATOM	2988	OH2	WAT	S1792	20.149	16.998	31.047	1.00	26.99	S
ATOM	2989	OH2	WAT	S1793	34.123	42.842	21.180	1.00	24.49	S
ATOM	2990	OH2	WAT	S1794	49.929	18.274	53.829	1.00	39.26	S
ATOM	2991	OH2	WAT	S1795	14.815	31.617	9.739	1.00	35.94	S
ATOM	2992	OH2	WAT	S1796	45.588	41.539	53.753	1.00	35.01	S
ATOM	2993	OH2	WAT	S1797	33.245	52.433	24.002	1.00	34.85	S
ATOM	2994	OH2	WAT	S1798	43.010	24.276	22.909	1.00	21.38	S
ATOM	2995	OH2	WAT	S1799	19.769	14.826	46.718	1.00	30.67	S
ATOM	2996	OH2	WAT	S1800	29.812	17.873	43.458	1.00	28.85	S
ATOM	2997	OH2	WAT	S1801	7.028	22.438	24.718	1.00	30.13	S
ATOM	2998	OH2	WAT	S1802	7.451	42.723	16.836	1.00	34.86	S
ATOM	2999	OH2	WAT	S1803	13.062	50.532	16.899	1.00	27.23	S
ATOM	3000	OH2	WAT	S1804	31.535	17.528	46.115	1.00	21.48	S
ATOM	3001	OH2	WAT	S1805	1.214	41.199	23.409	1.00	33.03	S
ATOM	3002	OH2	WAT	S1806	12.350	33.958	40.836	1.00	34.82	S
ATOM	3003	OH2	WAT	S1807	33.164	41.928	54.755	1.00	33.81	S
ATOM	3004	OH2	WAT	S1808	4.467	50.285	27.482	1.00	36.79	S
ATOM	3005	OH2	WAT	S1809	60.702	26.732	42.684	1.00	35.13	S
ATOM	3006	OH2	WAT	S1810	22.799	31.560	57.795	1.00	32.80	S
ATOM	3007	OH2	WAT	S1811	16.630	35.862	8.507	1.00	29.92	S
ATOM	3008	OH2	WAT	S1812	58.212	35.487	40.540	1.00	33.76	S
ATOM	3009	OH2	WAT	S1813	31.566	17.525	26.426	1.00	39.01	S
ATOM	3010	OH2	WAT	S1814	38.884	37.614	20.120	1.00	33.89	S
ATOM	3011	OH2	WAT	S1815	58.154	24.777	37.822	1.00	35.73	S
ATOM	3012	OH2	WAT	S1816	34.384	14.783	47.649	1.00	37.28	S
ATOM	3013	OH2	WAT	S1817	3.439	43.153	36.372	1.00	30.78	S
ATOM	3014	OH2	WAT	S1818	47.394	12.444	43.290	1.00	30.32	S
ATOM	3015	OH2	WAT	S1819	24.644	13.829	44.044	1.00	32.65	S
ATOM	3016	OH2	WAT	S1820	35.990	42.985	32.322	1.00	29.66	S
ATOM	3017	OH2	WAT	S1821	26.914	40.212	9.947	1.00	33.58	S
ATOM	3018	OH2	WAT	S1822	40.296	29.386	23.361	1.00	44.10	S
ATOM	3019	OH2	WAT	S1823	42.915	30.163	27.417	1.00	33.23	S
ATOM	3020	OH2	WAT	S1824	14.322	38.428	8.032	1.00	35.73	S
ATOM	3021	OH2	WAT	S1825	33.329	16.000	45.385	1.00	29.78	S
ATOM	3022	OH2	WAT	S1826	55.683	28.168	38.449	1.00	30.81	S
ATOM	3023	OH2	WAT	S1827	18.514	45.706	9.695	1.00	34.33	S
ATOM	3024	OH2	WAT	S1828	19.453	54.788	22.809	1.00	42.02	S
ATOM	3025	OH2	WAT	S1829	46.686	27.005	20.816	1.00	31.17	S
ATOM	3026	OH2	WAT	S1830	50.779	32.327	54.666	1.00	44.04	S
ATOM	3027	OH2	WAT	S1831	5.243	43.614	40.262	1.00	40.69	S
ATOM	3028	OH2	WAT	S1832	45.151	43.041	33.919	1.00	28.47	S
ATOM	3029	OH2	WAT	S1833	26.385	11.949	41.104	1.00	33.70	S
ATOM	3030	OH2	WAT	S1834	36.104	26.756	17.653	1.00	32.43	S
ATOM	3031	OH2	WAT	S1835	40.585	7.298	41.894	1.00	32.97	S
ATOM	3032	OH2	WAT	S1836	22.940	54.196	16.985	1.00	39.88	S
ATOM	3033	OH2	WAT	S1837	53.968	24.450	37.442	1.00	39.29	S
ATOM	3034	OH2	WAT	S1838	16.318	26.973	42.179	1.00	32.94	S
ATOM	3035	OH2	WAT	S1839	14.513	48.940	39.307	1.00	29.97	S

FIGURE 5 (continued)

45 / 46

ATOM	3036	OH2	WAT	S1840	31.652	6.945	51.493	1.00	27.66	S
ATOM	3037	OH2	WAT	S1841	41.996	11.677	38.039	1.00	37.88	S
ATOM	3038	OH2	WAT	S1842	7.510	48.642	19.668	1.00	35.11	S
ATOM	3039	OH2	WAT	S1843	42.467	3.493	49.912	1.00	33.41	S
ATOM	3040	OH2	WAT	S1844	59.776	22.501	42.412	1.00	44.37	S
ATOM	3041	OH2	WAT	S1845	7.867	44.473	12.687	1.00	34.20	S
ATOM	3042	OH2	WAT	S1846	15.405	45.353	39.658	1.00	38.08	S
ATOM	3043	OH2	WAT	S1847	13.585	15.183	28.501	1.00	36.58	S
ATOM	3044	OH2	WAT	S1848	48.442	41.492	47.985	1.00	26.95	S
ATOM	3045	OH2	WAT	S1849	50.374	40.886	46.017	1.00	34.93	S
ATOM	3046	OH2	WAT	S1850	44.568	8.030	45.822	1.00	42.34	S
ATOM	3047	OH2	WAT	S1851	48.705	28.443	22.632	1.00	34.87	S
ATOM	3048	OH2	WAT	S1852	38.217	33.408	18.268	1.00	40.91	S
ATOM	3049	OH2	WAT	S1853	26.698	47.866	16.749	1.00	26.87	S
ATOM	3050	OH2	WAT	S1854	36.624	40.405	57.361	1.00	30.57	S
ATOM	3051	OH2	WAT	S1855	44.243	22.209	21.682	1.00	25.97	S
ATOM	3052	OH2	WAT	S1856	50.807	22.291	30.826	1.00	30.01	S
ATOM	3053	OH2	WAT	S1857	2.113	19.175	16.420	1.00	39.64	S
ATOM	3054	OH2	WAT	S1858	35.799	20.261	25.717	1.00	29.95	S
ATOM	3055	OH2	WAT	S1859	10.845	51.013	18.474	1.00	29.30	S
ATOM	3056	OH2	WAT	S1860	13.036	16.982	18.603	1.00	35.56	S
ATOM	3057	OH2	WAT	S1861	48.755	33.466	53.529	1.00	32.19	S
ATOM	3058	OH2	WAT	S1862	28.542	12.640	28.777	1.00	32.37	S
ATOM	3059	OH2	WAT	S1863	15.582	33.781	40.294	1.00	31.38	S
ATOM	3060	OH2	WAT	S1864	15.389	51.736	31.264	1.00	35.97	S
ATOM	3061	OH2	WAT	S1865	59.586	24.576	44.154	1.00	38.45	S
ATOM	3062	OH2	WAT	S1866	33.931	18.197	52.470	1.00	31.45	S
ATOM	3063	OH2	WAT	S1867	33.400	24.810	14.487	1.00	31.43	S
ATOM	3064	OH2	WAT	S1868	2.939	39.474	28.464	1.00	42.13	S
ATOM	3065	OH2	WAT	S1869	52.149	36.661	45.439	1.00	34.90	S
ATOM	3066	OH2	WAT	S1870	45.901	34.119	54.146	1.00	28.55	S
ATOM	3067	OH2	WAT	S1871	21.485	29.372	44.666	1.00	37.03	S
ATOM	3068	OH2	WAT	S1872	10.455	19.175	23.705	1.00	36.18	S
ATOM	3069	OH2	WAT	S1873	29.820	54.141	17.625	1.00	37.56	S
ATOM	3070	OH2	WAT	S1874	36.824	12.036	41.616	1.00	36.62	S
ATOM	3071	OH2	WAT	S1875	35.575	29.695	13.582	1.00	31.58	S
ATOM	3072	OH2	WAT	S1876	47.689	26.645	56.483	1.00	29.75	S
ATOM	3073	OH2	WAT	S1877	25.923	24.021	7.877	1.00	35.32	S
ATOM	3074	OH2	WAT	S1878	35.914	42.663	19.444	1.00	38.13	S
ATOM	3075	OH2	WAT	S1879	53.553	27.199	37.462	1.00	34.02	S
ATOM	3076	OH2	WAT	S1880	31.012	18.989	51.960	1.00	32.14	S
ATOM	3077	OH2	WAT	S1881	5.543	24.207	39.126	1.00	33.92	S
ATOM	3078	OH2	WAT	S1882	12.515	49.450	14.280	1.00	38.32	S
ATOM	3079	OH2	WAT	S1883	19.621	34.441	42.264	1.00	32.10	S
ATOM	3080	OH2	WAT	S1884	0.567	34.443	15.606	1.00	41.76	S
ATOM	3081	OH2	WAT	S1885	19.842	21.597	48.228	1.00	38.20	S
ATOM	3082	OH2	WAT	S1886	17.245	44.489	41.443	1.00	36.34	S
ATOM	3083	OH2	WAT	S1887	31.241	17.703	18.315	1.00	43.85	S
ATOM	3084	OH2	WAT	S1888	47.120	35.974	31.511	1.00	44.95	S
ATOM	3085	OH2	WAT	S1889	16.721	12.447	25.646	1.00	42.81	S
ATOM	3086	OH2	WAT	S1890	17.002	21.309	47.530	1.00	35.74	S
ATOM	3087	OH2	WAT	S1891	11.124	36.224	11.415	1.00	28.23	S
ATOM	3088	OH2	WAT	S1892	31.476	35.439	12.666	1.00	29.98	S
ATOM	3089	OH2	WAT	S1893	20.313	44.798	8.239	1.00	38.49	S
ATOM	3090	OH2	WAT	S1894	49.492	37.692	31.490	1.00	34.21	S
ATOM	3091	OH2	WAT	S1895	11.168	48.631	11.775	1.00	35.00	S
ATOM	3092	OH2	WAT	S1896	8.149	35.174	12.830	1.00	43.18	S
ATOM	3093	OH2	WAT	S1897	42.985	36.028	29.277	1.00	37.84	S
ATOM	3094	OH2	WAT	S1898	15.722	26.088	38.269	1.00	40.56	S
ATOM	3095	OH2	WAT	S1899	9.466	42.584	43.325	1.00	38.58	S
ATOM	3096	OH2	WAT	S1900	55.683	27.859	55.011	1.00	40.16	S
ATOM	3097	OH2	WAT	S1901	16.412	44.824	6.088	1.00	35.00	S
ATOM	3098	OH2	WAT	S1902	30.819	20.863	13.376	1.00	36.12	S
ATOM	3099	OH2	WAT	S1903	20.083	45.050	40.249	1.00	46.55	S
ATOM	3100	OH2	WAT	S1904	55.216	16.767	37.256	1.00	32.34	S
ATOM	3101	OH2	WAT	S1905	17.194	15.633	31.289	1.00	41.92	S
ATOM	3102	OH2	WAT	S1906	55.468	39.305	45.956	1.00	33.48	S
ATOM	3103	OH2	WAT	S1907	34.073	59.171	22.880	1.00	29.68	S
ATOM	3104	OH2	WAT	S1908	11.696	23.487	37.533	1.00	44.83	S
ATOM	3105	OH2	WAT	S1909	37.193	57.700	24.645	1.00	29.20	S
ATOM	3106	OH2	WAT	S1910	4.958	20.071	12.971	1.00	38.75	S
ATOM	3107	OH2	WAT	S1911	28.212	15.651	46.090	1.00	44.28	S
ATOM	3108	OH2	WAT	S1912	25.791	17.881	50.101	1.00	44.07	S
ATOM	3109	OH2	WAT	S1913	44.830	16.225	28.015	1.00	37.34	S
ATOM	3110	OH2	WAT	S1914	45.538	25.603	58.524	1.00	31.60	S
ATOM	3111	OH2	WAT	S1915	31.849	53.832	20.135	1.00	44.08	S

FIGURE 5 (continued)

46 / 46

ATOM	3112	OH2	WAT	S1916	55.981	32.376	47.108	1.00	41.65	S
ATOM	3113	OH2	WAT	S1917	35.699	24.353	16.736	1.00	43.04	S
ATOM	3114	OH2	WAT	S1918	3.252	25.157	38.490	1.00	42.38	S
ATOM	3115	OH2	WAT	S1919	34.711	10.496	39.861	1.00	36.97	S
ATOM	3116	OS4	PLA	P1001	8.781	29.613	10.689	1.00	35.34	P
ATOM	3117	S2	PLA	P1001	9.783	28.546	11.256	1.00	33.57	P
ATOM	3118	OS5	PLA	P1001	10.409	27.663	9.867	1.00	40.37	P
ATOM	3119	OS6	PLA	P1001	11.159	29.189	12.135	1.00	41.03	P
ATOM	3120	C15	PLA	P1001	9.058	27.351	12.199	1.00	30.49	P
ATOM	3121	C14	PLA	P1001	7.662	27.126	12.015	1.00	23.35	P
ATOM	3122	C16	PLA	P1001	9.978	26.532	12.898	1.00	28.94	P
ATOM	3123	C10	PLA	P1001	9.499	25.436	13.634	1.00	30.90	P
ATOM	3124	C11	PLA	P1001	8.025	25.127	13.485	1.00	25.22	P
ATOM	3125	C13	PLA	P1001	7.134	25.968	12.614	1.00	21.41	P
ATOM	3126	O3	PLA	P1001	5.837	25.588	12.437	1.00	24.00	P
ATOM	3127	C12	PLA	P1001	7.519	23.932	14.212	1.00	27.53	P
ATOM	3128	O2	PLA	P1001	6.235	23.585	13.967	1.00	21.97	P
ATOM	3129	C9	PLA	P1001	10.366	24.618	14.415	1.00	32.13	P
ATOM	3130	C8	PLA	P1001	9.876	23.541	15.205	1.00	31.56	P
ATOM	3131	S1	PLA	P1001	10.846	22.324	15.981	1.00	31.16	P
ATOM	3132	OS3	PLA	P1001	12.358	22.881	16.679	1.00	39.44	P
ATOM	3133	OS2	PLA	P1001	11.138	21.153	14.733	1.00	28.72	P
ATOM	3134	OS1	PLA	P1001	10.061	21.436	17.011	1.00	39.17	P
ATOM	3135	C7	PLA	P1001	8.424	23.154	15.086	1.00	20.93	P
ATOM	3136	N2	PLA	P1001	7.947	21.974	15.652	1.00	27.49	P
ATOM	3137	N1	PLA	P1001	6.731	21.270	15.708	1.00	26.74	P
ATOM	3138	C2	PLA	P1001	6.780	19.948	16.206	1.00	29.90	P
ATOM	3139	C1	PLA	P1001	7.938	19.230	16.659	1.00	26.11	P
ATOM	3140	C3	PLA	P1001	5.455	19.218	16.215	1.00	29.97	P
ATOM	3141	O1	PLA	P1001	4.329	19.881	15.839	1.00	27.77	P
ATOM	3142	C4	PLA	P1001	5.419	17.867	16.622	1.00	27.79	P
ATOM	3143	C5	PLA	P1001	6.617	17.226	17.060	1.00	24.04	P
ATOM	3144	C6	PLA	P1001	7.890	17.875	17.105	1.00	28.93	P
ATOM	3145	CL1	PLA	P1001	8.958	17.179	17.619	1.00	13.83	P
ATOM	3146	OS4	PLA	P1002	-1.265	32.010	14.293	1.00	40.73	P
ATOM	3147	S2	PLA	P1002	-2.593	31.401	14.907	1.00	34.43	P
ATOM	3148	OS5	PLA	P1002	-3.293	32.318	16.225	1.00	36.70	P
ATOM	3149	OS6	PLA	P1002	-3.702	31.417	13.545	1.00	38.28	P
ATOM	3150	C15	PLA	P1002	-2.360	29.762	15.366	1.00	37.51	P
ATOM	3151	C14	PLA	P1002	-1.339	29.023	14.693	1.00	32.35	P
ATOM	3152	C16	PLA	P1002	-3.324	29.136	16.198	1.00	32.13	P
ATOM	3153	C10	PLA	P1002	-3.227	27.770	16.534	1.00	32.57	P
ATOM	3154	C11	PLA	P1002	-2.159	26.968	15.824	1.00	27.55	P
ATOM	3155	C13	PLA	P1002	-1.219	27.623	14.849	1.00	32.76	P
ATOM	3156	O3	PLA	P1002	-0.300	26.897	14.135	1.00	26.73	P
ATOM	3157	C12	PLA	P1002	-2.103	25.533	16.170	1.00	29.76	P
ATOM	3158	O2	PLA	P1002	-1.093	24.861	15.620	1.00	19.01	P
ATOM	3159	C9	PLA	P1002	-4.076	27.177	17.503	1.00	28.28	P
ATOM	3160	C8	PLA	P1002	-4.072	25.777	17.756	1.00	30.57	P
ATOM	3161	S1	PLA	P1002	-4.937	25.049	19.065	1.00	30.09	P
ATOM	3162	OS3	PLA	P1002	-6.417	25.925	19.382	1.00	26.32	P
ATOM	3163	OS2	PLA	P1002	-3.886	25.328	20.444	1.00	39.20	P
ATOM	3164	OS1	PLA	P1002	-5.060	23.483	18.960	1.00	35.43	P
ATOM	3165	C7	PLA	P1002	-3.056	24.884	17.116	1.00	30.01	P
ATOM	3166	N2	PLA	P1002	-2.942	23.547	17.510	1.00	30.83	P
ATOM	3167	N1	PLA	P1002	-1.994	22.600	17.132	1.00	26.11	P
ATOM	3168	C2	PLA	P1002	-2.109	21.347	17.777	1.00	33.57	P
ATOM	3169	C1	PLA	P1002	-3.069	20.979	18.767	1.00	28.55	P
ATOM	3170	C3	PLA	P1002	-1.126	20.289	17.352	1.00	32.70	P
ATOM	3171	O1	PLA	P1002	-0.254	20.633	16.366	1.00	26.71	P
ATOM	3172	C4	PLA	P1002	-1.181	19.011	17.978	1.00	35.63	P
ATOM	3173	C5	PLA	P1002	-2.175	18.727	18.965	1.00	32.99	P
ATOM	3174	C6	PLA	P1002	-3.137	19.696	19.364	1.00	34.82	P
ATOM	3175	CL1	PLA	P1002	-4.110	19.418	20.286	1.00	26.50	P
ATOM	3176	P	PO4	I1000	31.378	36.578	34.442	1.00	7.30	I
ATOM	3177	O1	PO4	I1000	30.121	37.237	34.900	1.00	8.97	I
ATOM	3178	O2	PO4	I1000	32.276	37.583	33.795	1.00	6.24	I
ATOM	3179	O3	PO4	I1000	31.043	35.497	33.462	1.00	6.45	I
ATOM	3180	O4	PO4	I1000	32.089	35.965	35.624	1.00	7.79	I
ATOM	3181	U	U	I1100	0.273	22.910	15.547	1.00	30.28	I
ATOM	3182	U	U	I1101	4.450	22.112	14.520	1.00	29.14	I
ATOM	3183	U	U	I1102	2.292	24.635	12.979	0.50	39.41	I
ATOM	3184	NA	NA	I1200	37.019	13.768	54.963	1.00	21.53	I
END										

FIGURE 5 (continued)